Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Synthesis of Well-defined Yttrium-based Lewis Acids by Capture of a Reaction Intermediate and Catalytic Application for Cycloaddition of CO_2 to Epoxides Under Atmospheric Pressure

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S1: *General information*

All materials were sourced from commercial suppliers (Merck or Alfa Aesar, unless otherwise stated). All operation involving air-sensitive materials were conducted under nitrogen atmosphere using standard Schlenk techniques, or in a glovebox. All solvents were initially dried using a Pure Process Technology solvent purification system and degassed by freeze-pump-thaw cycles on a high vacuum line. Dichloromethane was stored over 4 Å molecular sieves under an atmosphere of solvent vapor. Deuterated solvents were purchased from Cambridge Isotope Laboratories and were degassed by freeze-pump-thaw cycles on a high vacuum line, dried over 4 Å molecular sieves and then stored under a nitrogen atmosphere. Propylene oxide was distilled before use, degassed by freeze-pump-thaw cycles on a high vacuum line and then stored under an nitrogen atmosphere. Partially dehydroxylated silica was prepared from Aerosil 200 (Evonik, specific area 200 m^2/g), dehydroxylated for 18 hours under dynamic high vacuum (10^{-5} mbar at 700 °C ($SiO_{2\text{-}700}$)) or under 10^{-3} mbar at 200 °C (tt-SiO_2). Carbon dioxide 99.999% and nitrogen (Ultra high pure, 99.999%) form Bangkok Industrial Gas Company Ltd. were used as supplied.

Infrared Spectroscopy. IR spectra were recorded on a PerkinElmer Frontier FT-IR spectrometer (Universal-ATR model) equipped with a cell for transmission mode measurements under protective atmosphere. Moisture sensitive materials were blended with dry KBr and pressed in a pellet. Typically, 16 scans were accumulated for each spectrum (resolution = 4 cm^{-1}).

Elemental analysis.

CHN determination: CHN content was determined using a Leco TruSpec Micro Elemental Series CHNS analyzer using tin capsules for loading the samples.

Determination of Y and halide content: For determination of yttrium (ICP-OES) and halide (Mohr's method) content the prepared materials were digested beforehand in nitric acid: 20 mg of material was suspended in 65 wt% nitric acid (3 mL) and the mixture was stirred for 12 h at 95 °C . Subsequently, deionized water was added up to 100 mL final volume. Residual solid particles were removed by filtration. The amount of yttrium in the sample was determined by Agilent Technologies 710 Series ICP-OES against a standard calibration curve prepared using variable concentrations of YCl_3. The total amount of halides (chloride plus bromide) was determined according to Mohr's method: after digestion as described above, the digestion solution was diluted by addition of deionized water up 50 mL final volume. 1 M NaOH solution was added to the diluted digestion solution until reaching pH = 9. K_2CrO_4 solution (0.25 M, 1 mL) was added as indicator. Finally, the resulting solution was titrated by dropwise addition of 0.01 M $AgNO_3$ solution until the color of the indicator changed from yellow to red-brown. The titration experiment was repeated three times and the results were averaged.

X-ray photoelectron spectroscopy (XPS) was recorded on JEOL JPS-9010MC with a Mg Kα source (1253.6 ev) at 12 kV and 25 mA. All XPS spectra were measured under high vacuum (10^{-8} Pa) at a room temperature using the software SpecSurf 1.9.3. For the experiments, carbon tape was coated with powder samples. The analyzed area of each sample was a circle spot with diameter of 6 mm. The survey scan spectra were measured with a pass energy of 50 eV, a binding energy range of 0-1100 eV and an electron-volt step of 1 eV. The obtained spectra were evaluated using JEOL software to obtain the chemical state of the probing elements and elemental composition. All the binding energy values were referenced to the carbon peak C 1s at 284.70 eV.

Liquid-State Nuclear Magnetic Resonance Spectroscopy. All liquid-state NMR spectra were recorded on a Bruker Advance III 600 MHz spectrometer, using $CDCl_3$ and DMSO-D_6 as the solvent. All chemical shifts were measured relative to the internal standard tetramethyl silane (TMS; ^1H or ^{13}C resonances appear at 0.00 ppm) present in $CDCl_3$.

Solid-State Nuclear Magnetic Resonance Spectroscopy. One dimensional ^1H MAS, ^{13}C CP/MAS solid state NMR spectra were recorded on a Bruker AVANCE III spectrometer operating at 400 and 100 MHz resonance frequencies for ^1H and ^{13}C respectively, with a conventional double resonance 4 mm CP/MAS probe. The samples were introduced under argon into zirconia rotors, which were then tightly closed. The spinning frequency was set to 15 and 10 KHz for ^1H and ^{13}C respectively. NMR chemical shifts are reported with respect to TMS as an external reference. For CP/MAS ^{13}C, the following sequence was used: 900 pulse on the proton (pulse length 2.4 s), then a cross-polarization step with a contact time typically 2 ms, and finally acquisition of the ^{13}C signal under high power proton decoupling. The delay between the scan was set to 4 s, to allow the complete relaxation of the ^1H nuclei and the number of scans was between 10,000 for carbon and 16 for proton. An apodization function (exponential) corresponding to a line broadening of 80 Hz was applied prior to Fourier transformation.

Scanning electron microscopy/Energy Dispersive X-Ray Spectroscopy (SEM/EDX) morphology images and compositional analysis mapping were acquired using a JEOL JSM-7610F field emission scanning electron microscope equipped with an Oxford Instruments EDS. The samples were spread over carbon tape and attached to the sample holder without platinum sputtering.

High resolution transmission electron microscopy (HRTEM) along with scanning transmission electron microscopy (STEM) and energy dispersive X-ray spectroscopy (EDS) mapping were acquired by a JEOL-ARM200F system. Samples were prepared by dispersing the catalysts powder in dichloromethane and by dipping the TEM grid (Ultrathin C Type-A 400 mesh, Cu by Ted Pella) in the suspension.

X-ray absorption spectroscopy (XAS). **X-ray absorption spectroscopy (XAS)** experiments were performed on the beamline 5.2: SUT-NANOTEC-SLRI XAS at the synchrotron light research institute (SLRI) facility in Nakhon-Ratchasima, Thailand. XANES spectra were measured at the yttrium L_3-edge (2080 eV), from 30 eV before the edge to 80 eV above the edge. The details of the beamline and its optical devices were described earlier.[1] The incident (I0) and transmitted (I1) intensities were measured by ionization chambers. The fluorescence photons were measured by a 4-element silicon drift detector. All XANES data were analyzed using the Athena program of the IFEFFIT package.[2] The XANES spectra were obtained after performing standard procedures for pre-edge subtraction, and normalization.

Kinetic measurements (*in situ* IR): The experiments were carried out in a stainless-steel autoclave equipped with an inlet for *in situ* ATR-IR probe. The *in situ* IR measurements were carried out using a Mettler Toledo ReactIR™ 15 with MCT detector using Happ-Genzel apodization. The evolution of the IR signal at 1810 cm^{-1}, relative to cyclic carbonate evolution ($\nu_{C=O}$), was monitored for the initial 15 min of reaction by collecting an IR spectrum every minute. After a short induction period (2-3 min), data points relative to the height of the carbonate peak versus time were fitted with linear regression obtaining the apparent initial rate (k_{obs}) as the slope of the curve. k_{obs} values are given in arbitrary units (a. u.) because include an instrumental response factor. Further mathematical treatment of kinetic data collected by *in situ* IR is provided elsewhere[3] in the supporting information.

S2: *Supporting IR and NMR spectra*

Raw solution phase ^{1}H (Figure S1), ^{13}C NMR (Figure S2) and bidimensional (2D) ^{1}H-^{1}H correlation NMR (COSY) spectra (Figure S3) of **I** were measured by mixing equimolar amounts of YCl_3 (214.8 mg, 1.1 mmol), TBAB (354.6 mg, 1.1 mmol) and 2 equivalents of propylene oxide (154 µL, 2.2 mmol). The mixture was stirred for 3 h until obtaining a clear solution. After this period, DCM was removed by evaporation under reduced pressure to yield a white solid. An aliquot of this solid was dissolved in DMSO-d6 without further purification for NMR measurement.

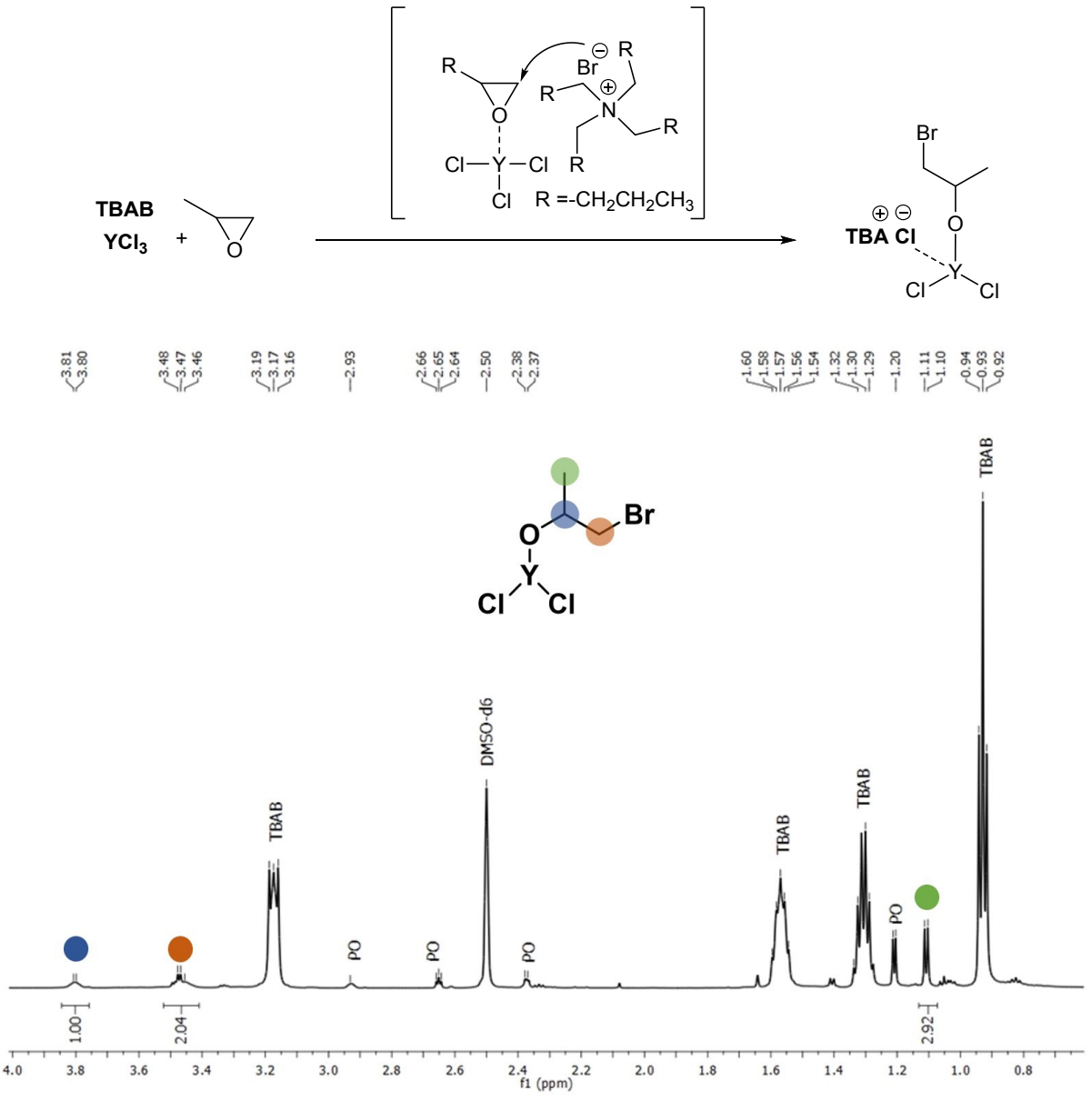


Figure S1. ^{1}H NMR spectrum of **I** in DMSO-d6. The protons of the opened epoxide ring are color-coded as shown in the structure in the inset.

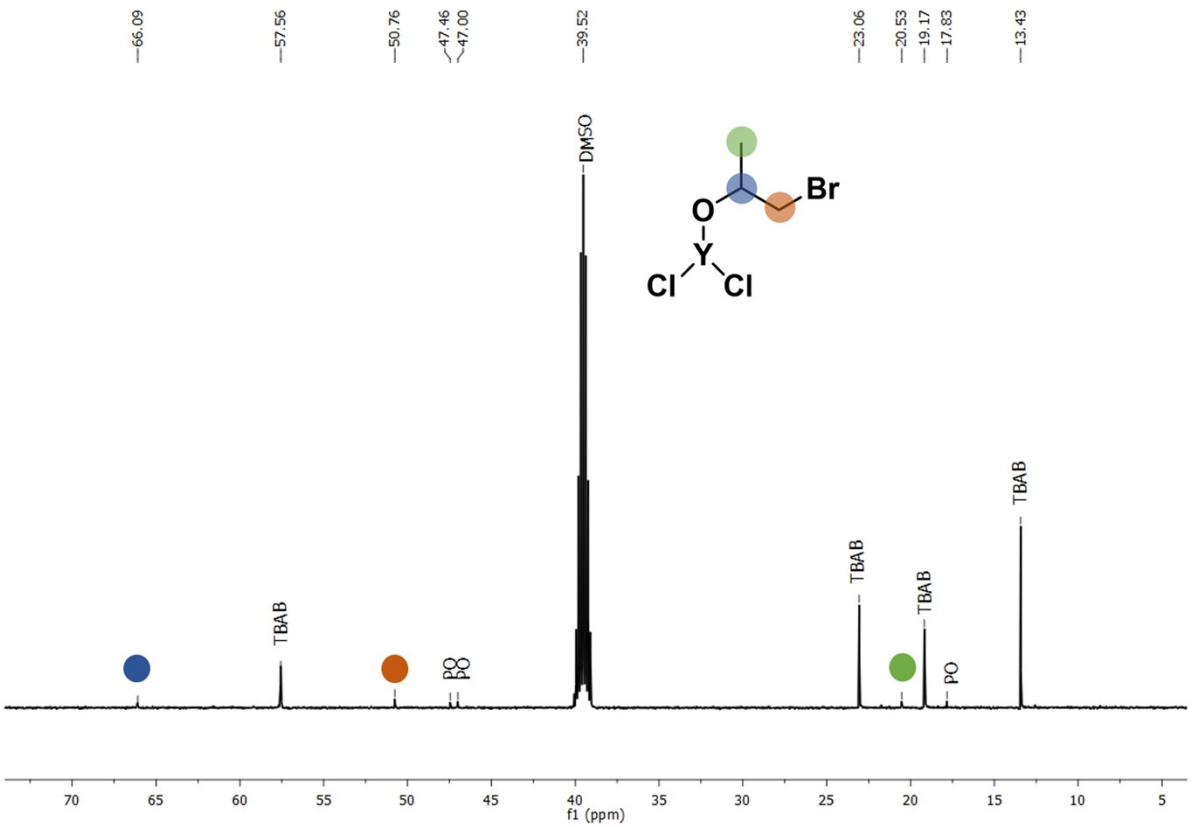


Figure S2. ^{13}C NMR spectrum of **I** in DMSO-d6. The carbon atoms of the opened epoxide ring are color-coded as shown in the structure in the inset.

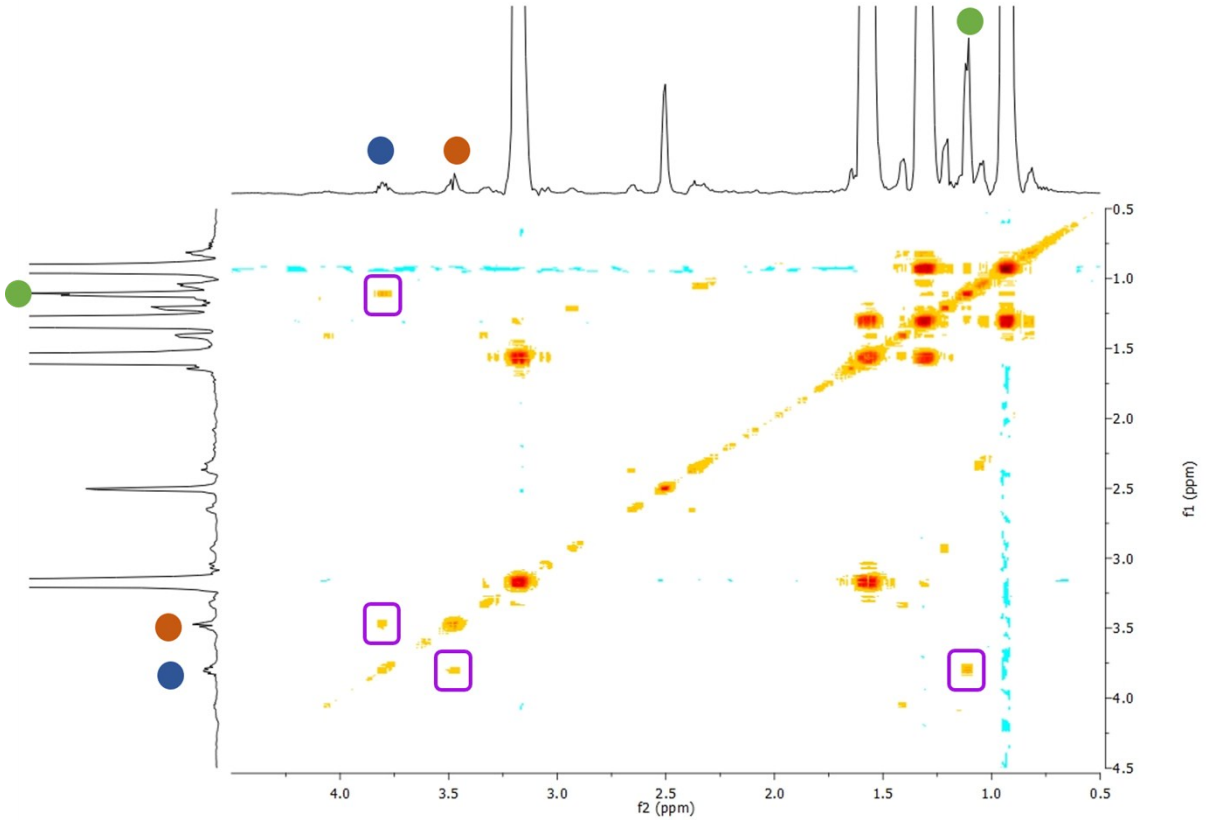


Figure S3. 2D ^{1}H-^{1}H COSY spectrum of **I** in DMSO-d6 highlighting the correlation between the protons of the ring-opened epoxide.

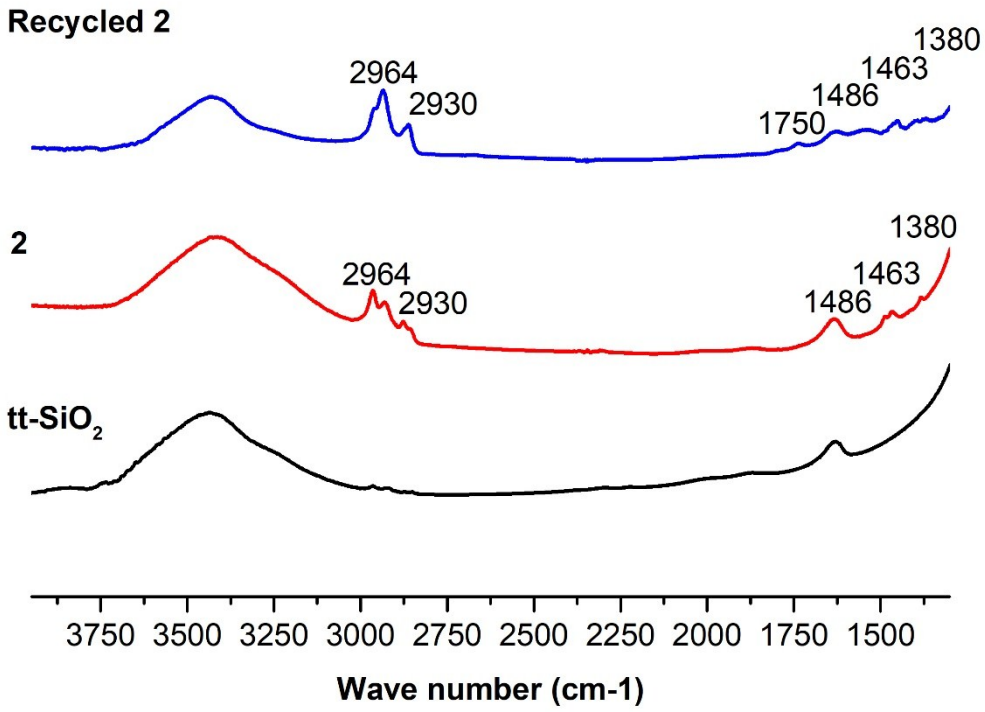


Figure S4. FT-IR spectra of tt-SiO_2 (black trace, bottom), material **2** (red trace, middle) and material **2** after three catalytic cycles (top).

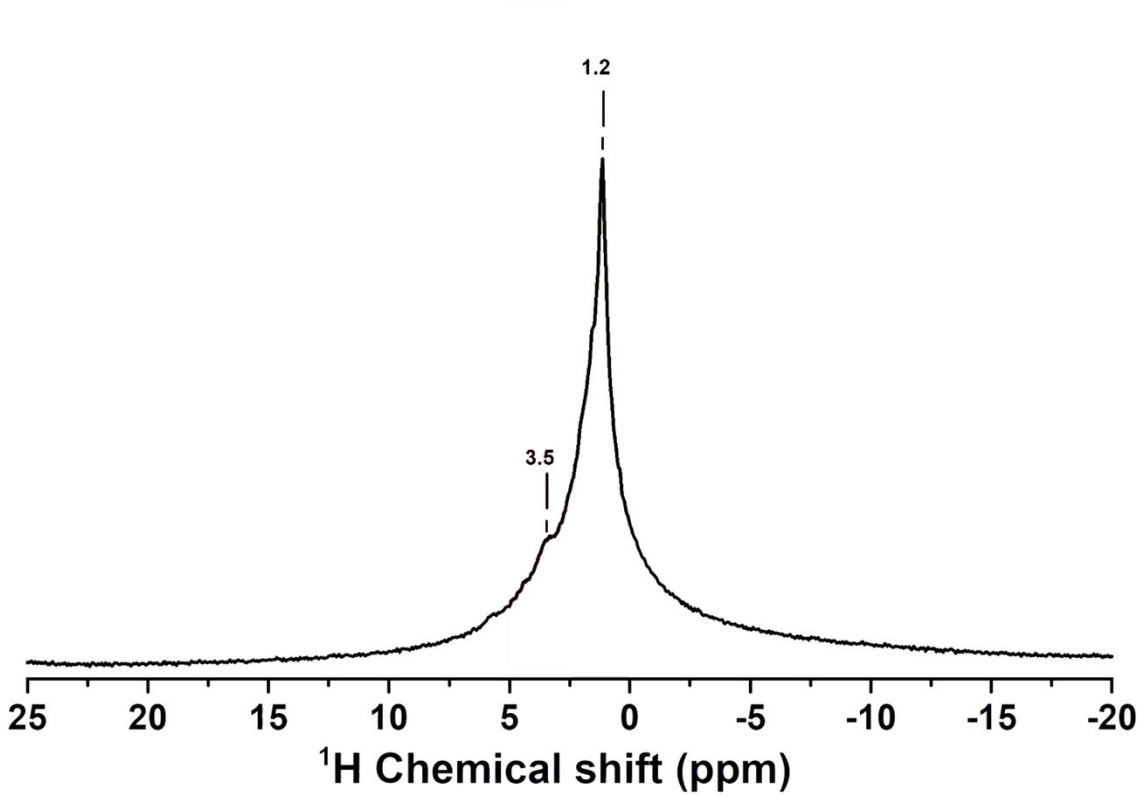


Figure S5. Solid state ^{1}H-NMR spectrum of **1** showing presence of the signals relative to the quaternary ammonium moiety.

S3: *XPS characterization and quantification*

High resolution XPS spectra have been fitted with JEOL Analysis software using Shirley type background and Voigt lineshapes. The element quantification in terms of atomic fraction (At%) was carried out by the software basing on Cl $2p_{3/2}$, Br $3d_{5/2}$ and Y $3d_{5/2}$ peaks area and utilizing the relative sensitivity factors. Cl and Br 2p and 3d peaks were respectively fitted by two peaks representing $2p_{1/2}$ and $2p_{3/2}$ for Cl and $3d_{3/2}$ and $3d_{5/2}$ for Br. Y 3d peak was fitted with 2 peaks accounting the spin orbit interaction, namely $3d_{3/2}$ and $3d_{5/2}$, however it was necessary to deconvolute it from the Si 2s peak occurring at 153.4 eV. In order to properly fit Si 2s peak, three evenly spaced peaks accounting for the existence of different oxidation states[4] of Si were introduced giving rise to a shoulder at around 154 eV. The 2s satellite peak at 145 eV was also deconvoluted from this portion of the spectrum.

As measured atomic ratios, namely Y/Cl and Cl/Br, were corrected by relative sensitivity factors (RSF) extracted from XPS atomic quantification of 99.999 % YCl_3 and 99.999 % YBr_3. The empirical RSF ratios ($F_{Y/X}$) were calculated as:

$$F_{Y/X} = \frac{(At\%)_X}{(At\%)_Y}\frac{1}{3}$$

With X=Cl,Br, obtaining $F_{Y/Cl} = 0.34$ and $F_{Y/Br} = 0.60$ respectively. The (Cl At%)/(At% Br) ratio was calculated as follow: $R_{Cl/Br} = \frac{(At\%)_{Cl}}{(At\%)_{Br}}\frac{F_{Y/Br}}{F_{Y/Cl}}$

These correction factors are close but slightly different than those calculated from the literature RSF values, i.e. 0.41 for Y-Cl and 0.52 for Y-Br respectively.[5] However, the calculation of correction factors relative to the instrument used is preferable.[6]

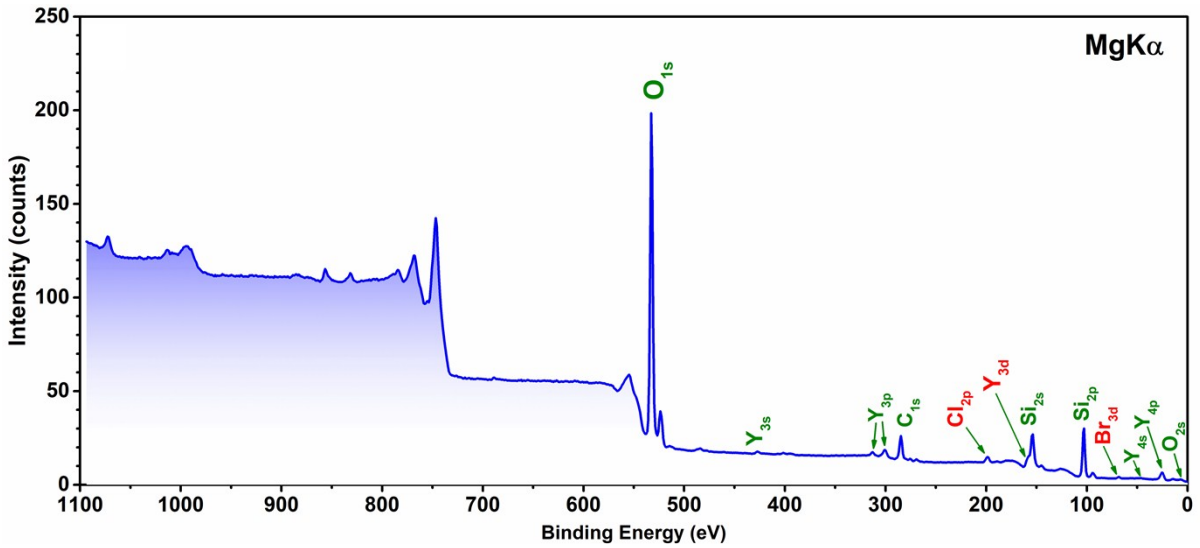


Figure S6. Survey XPS spectrum of **1.** For high-resolution spectra see Figure 3 of the manuscript.

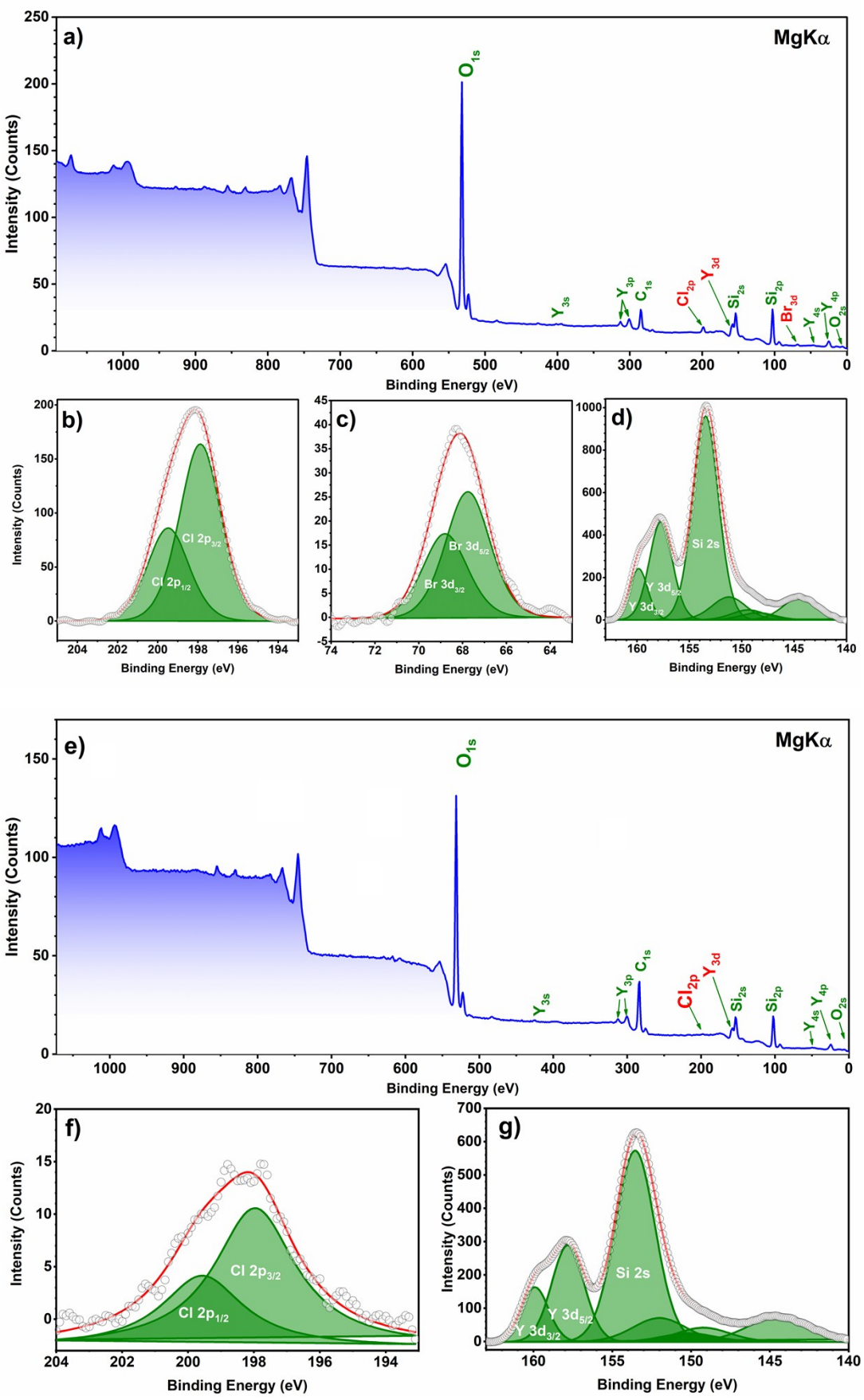


Figure S7. Surveys (a, e) and excerpts (b, c, d, f, g) of the high-resolution XPS spectra of pristine **2** (a-d) and recovered **2** (e-g) after three catalytic cycles.

Table S1. Pristine and corrected element quantization in terms of atomic percentage (at%) from deconvoluted XPS spectra.

Material	Y at%[a]	Cl at%[a]	Br at%[a]	Cl/Y	Cl/Y corrected	Cl/Br	Cl/Br corrected
1	60.0	32.6	7.4	0.54	1.58	4.41	7.6
2	61.3	32.2	6.5	0.52	1.52	4.96	8.6
2[b]	90.3	9.7	-	0.11	0.32	-	-

[a] Atomic percentages relative to the combined amounts of Y, Cl, Br in the samples.

[b] Spent catalyst.

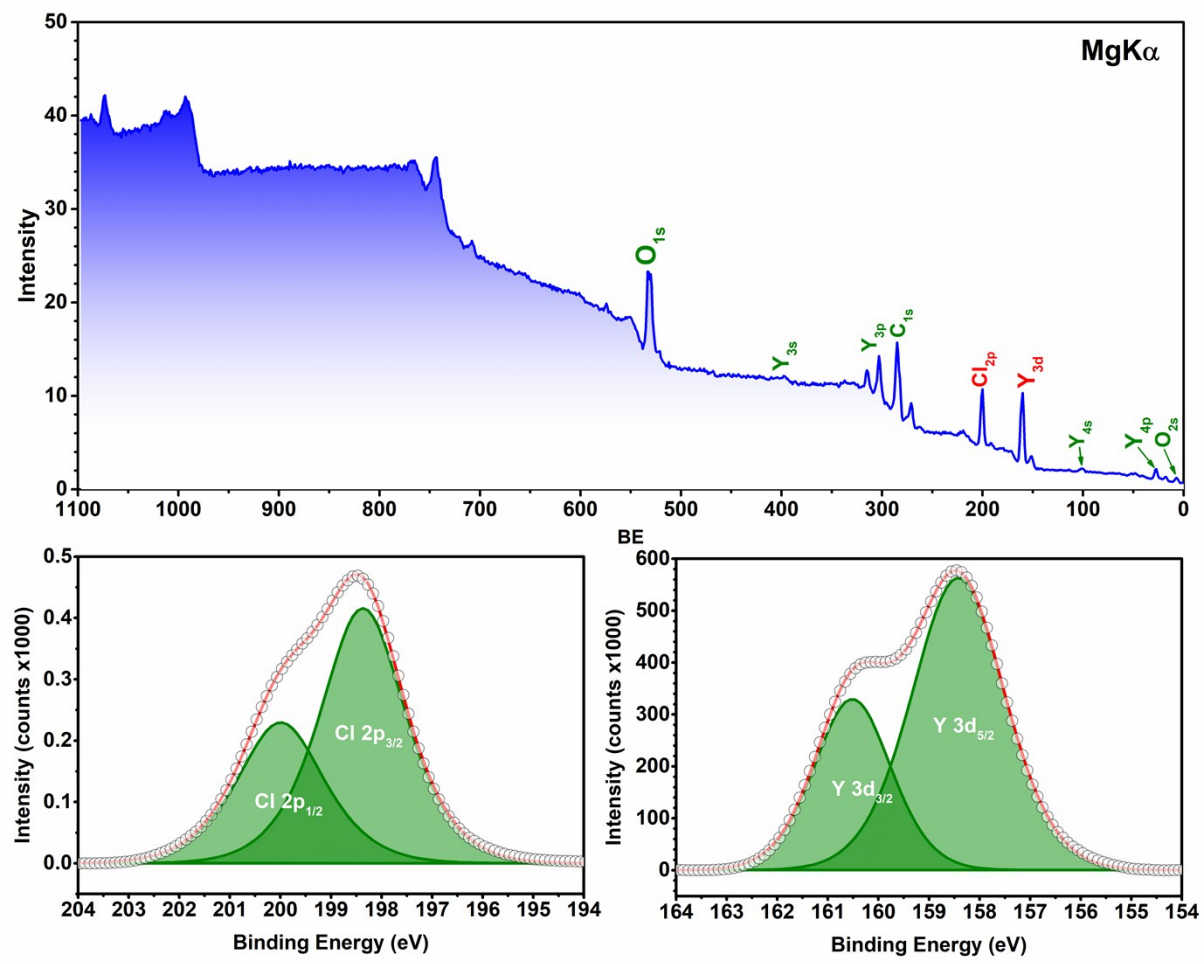


Figure S8. Survey (top) and excerpts of high-resolution XPS spectrum (bottom) of anhydrous YCl_3.

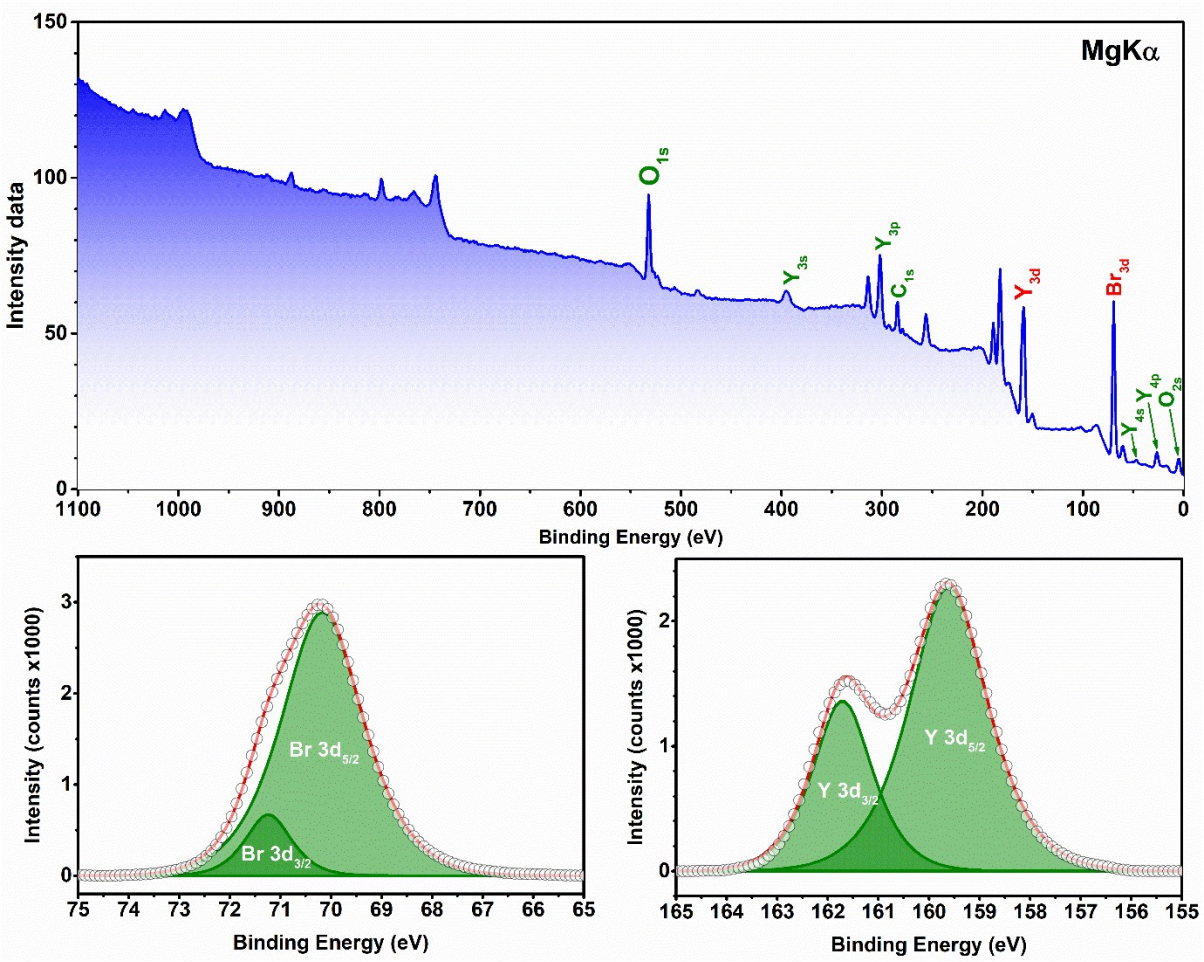


Figure S9. Survey (top) and excerpts of high-resolution XPS spectrum (bottom) of anhydrous YBr_3.

Table S2. Binding energy of deconvoluted peaks of samples **1**, **2**, YCl_3 and YBr_3. The binding energies are customarily expressed in eV.

Sample	$Y3d_{3/2}$	$Y3d_{5/2}$	$Cl2p_{1/2}$	$Cl2p_{3/2}$	$Br3d_{3/2}$	$Br3d_{5/2}$
YCl_3	161.98	159.88	201.62	200.02	-	-
YBr_3	161.71	159.61	-	-	69.92	70.96
1	159.94	157.77	199.45	197.85	67.60	68.64
2	159.84	157.72	199.48	197.88	67.76	68.80
2[a]	159.91	157.82	199.57	197.97	-	-

[a] Spent catalyst.

S4: *XANES spectroscopy*

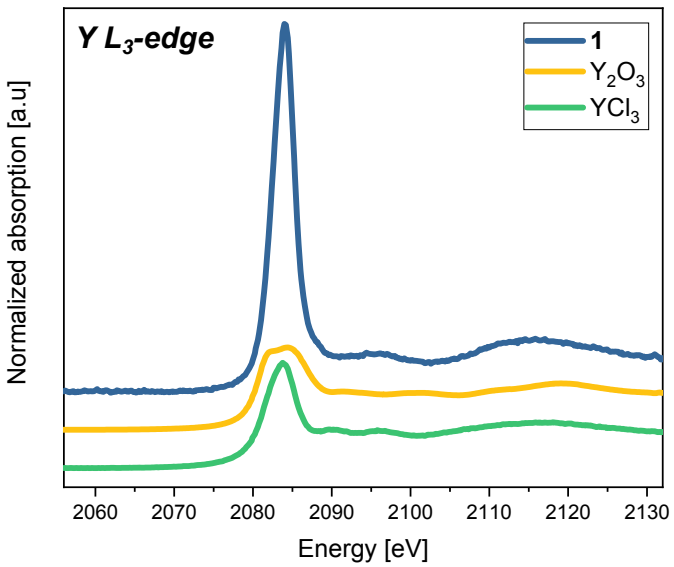


Figure S10: XANES spectra measured at the Y L_3-edge for compound **1** with Y_2O_3 and YCl_3 references. The spectra have been normalized and shifted for the sake of clarity.

S5: ***SEM and TEM micrographs***

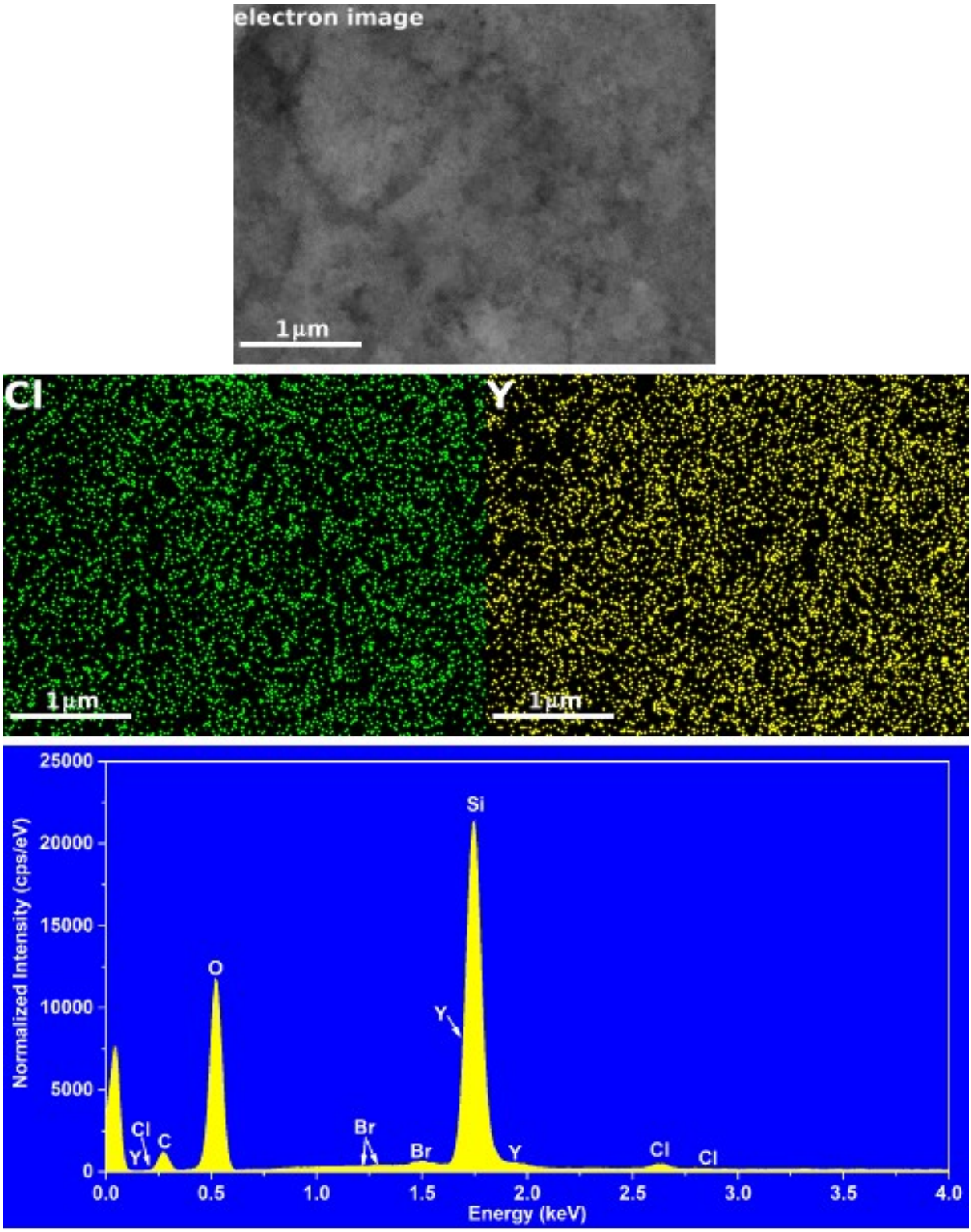


Figure S11. (top) electron image, (center) Y and Cl EDS mappings and (bottom) EDS Spectrum of **1.**

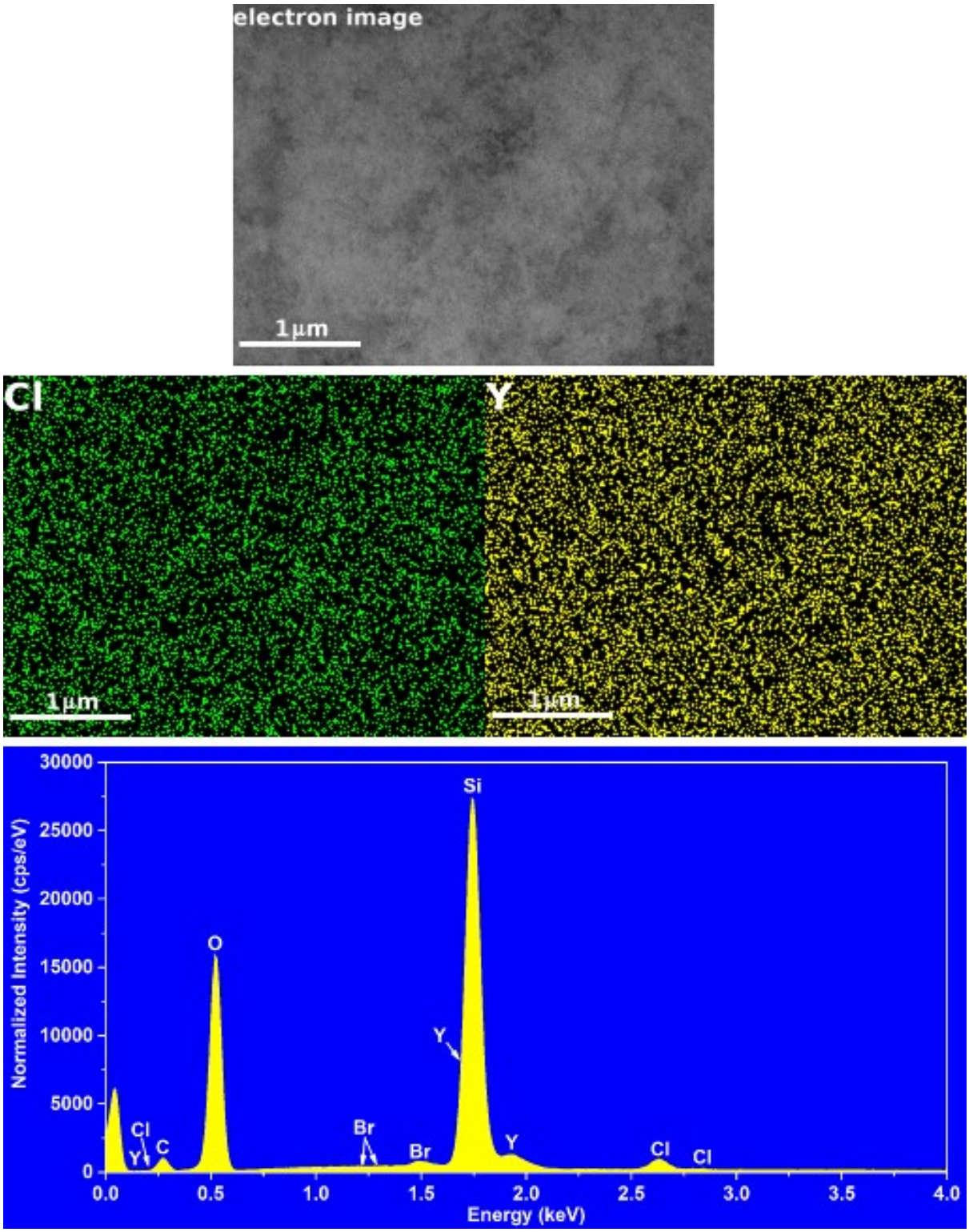


Figure S12. (top) electron image, (center) Y and Cl EDS mappings and (bottom) EDS spectrum of **2.**

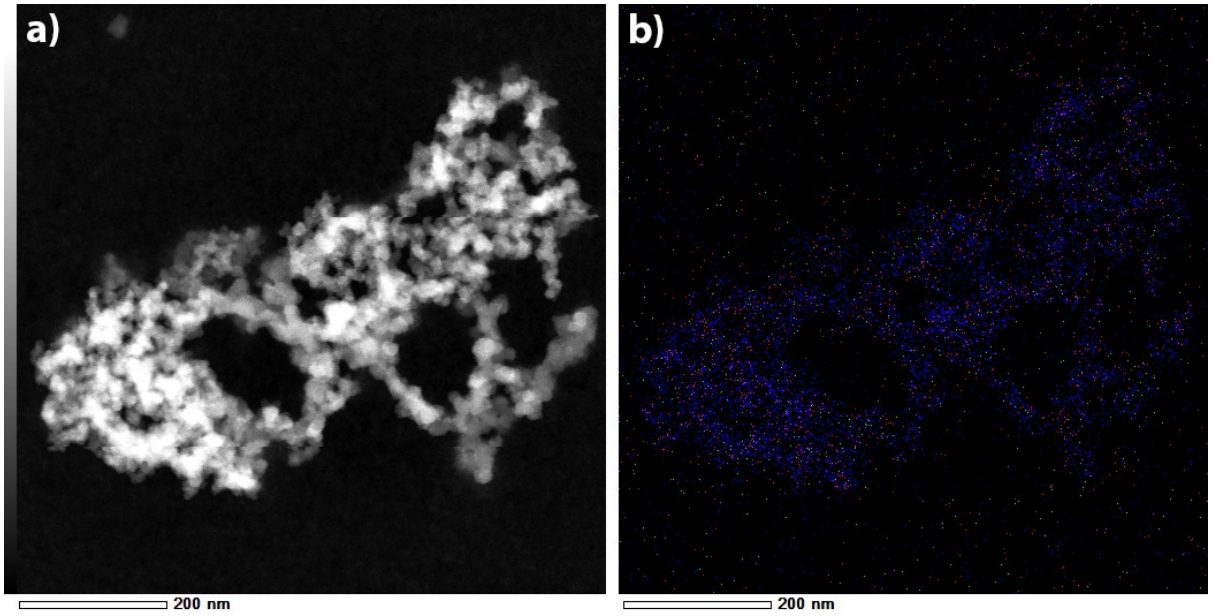


Figure S13. a) ADF-TEM image and b) EDS mapping (Si (blue), Y (red) and Cl (green)) of material **2**.

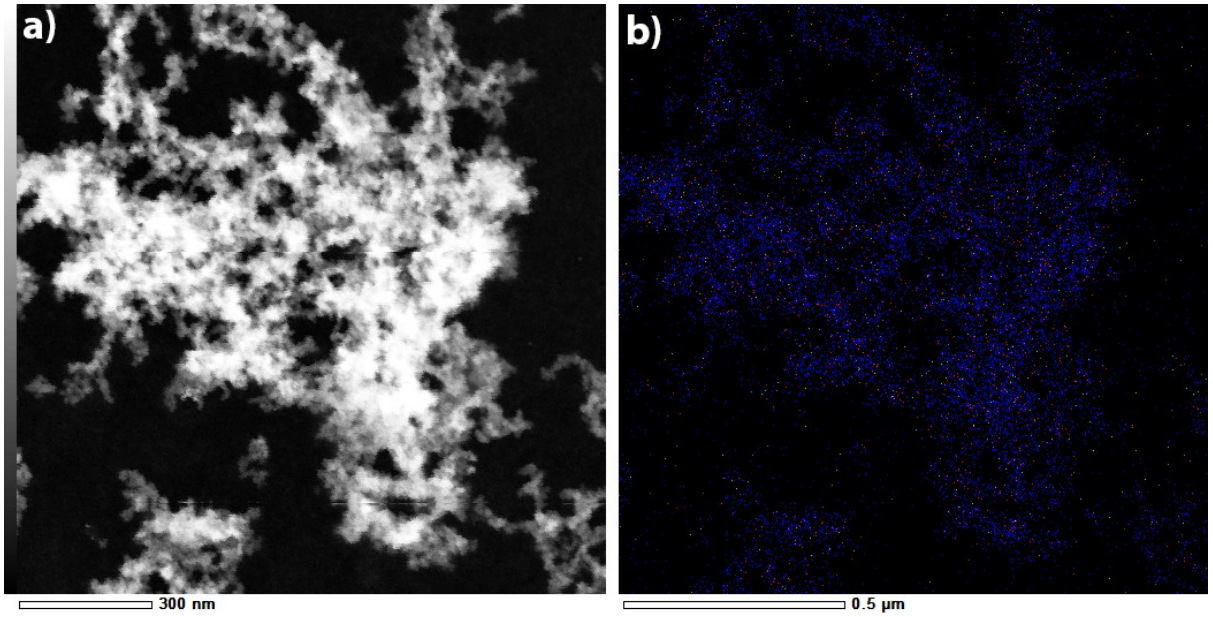


Figure S14. a) ADF-TEM image and b) EDS mapping (Si (blue), Y (red) and Cl (green)) of material **2** after three catalytic cycles.

S6: *^{1}H NMR Spectra of catalytic reactions (CO_2-cycloaddition)*

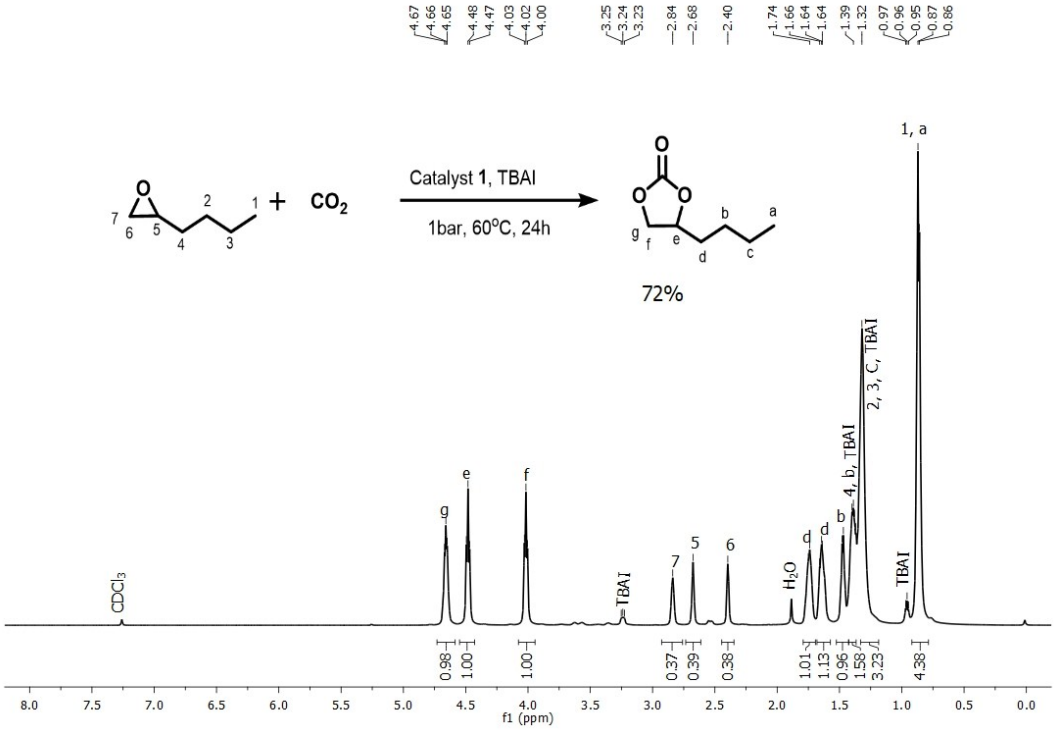


Figure S15. Crude ^{1}H-NMR spectra of cycloaddition of CO_2 to 1,2-Epoxyhexane by using catalyst **1** with TBAI (Table 3, Entry 1).

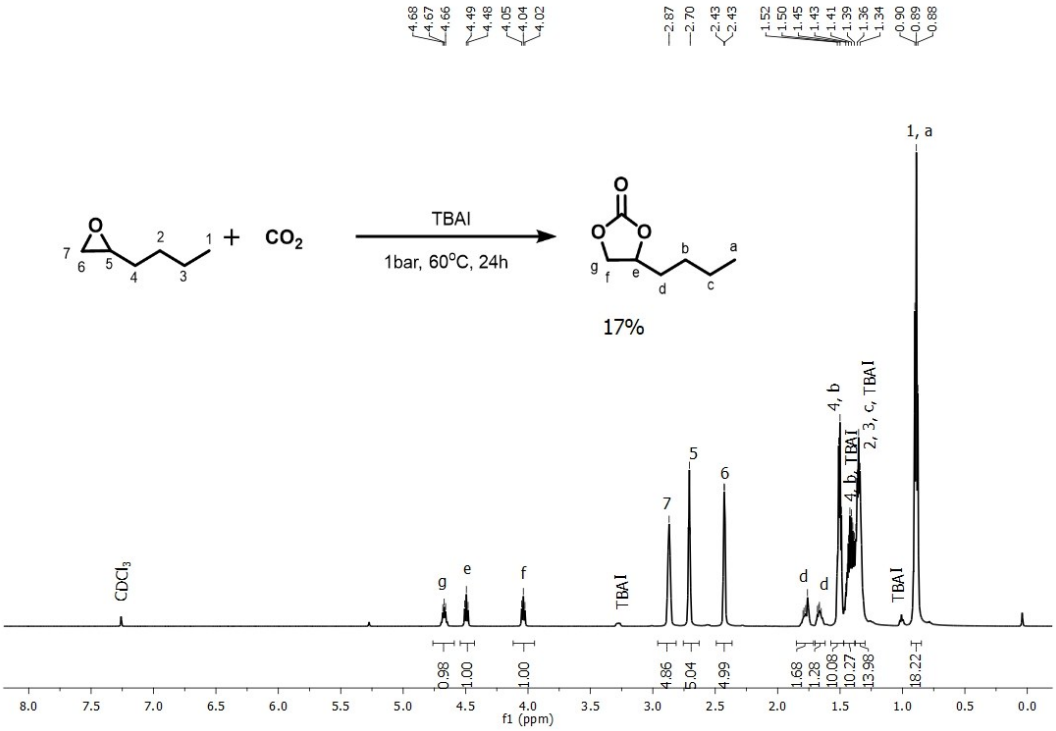


Figure S16. Crude ^{1}H-NMR spectra of cycloaddition of CO_2 to 1,2-Epoxyhexane by using only TBAI (Table 3, Entry 2).

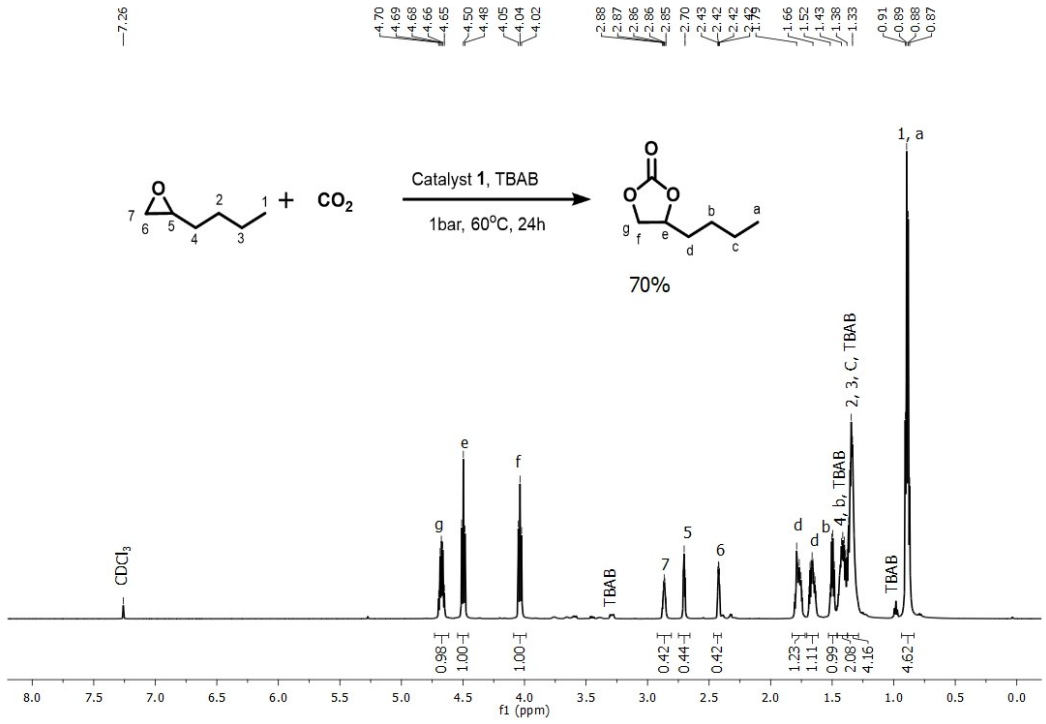


Figure S17. Crude ^{1}H-NMR spectra of cycloaddition of CO_2 to 1,2-Epoxyhexane by using catalyst **1** with TBAB (Table 3, Entry 3).

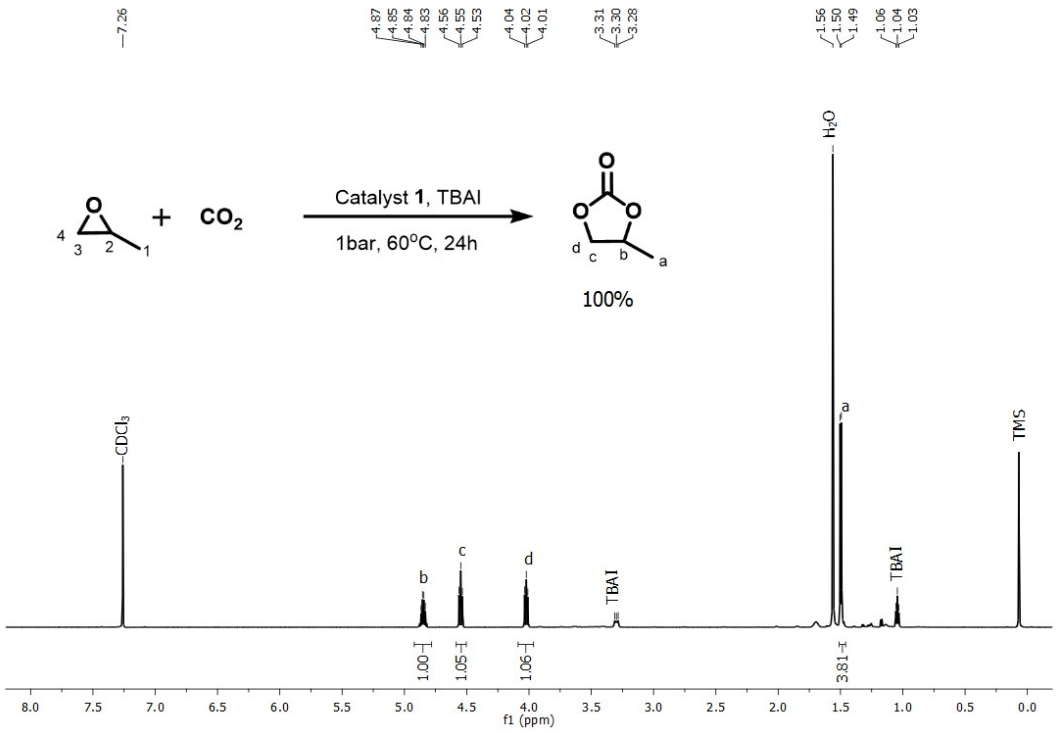


Figure S18. Crude ^{1}H-NMR spectra of cycloaddition of CO_2 to Propylene oxide by using catalyst **1** with TBAI. The $CDCl_3$ solvent used for this spectrum contains water and TMS as standards (Table 3, Entry 4).

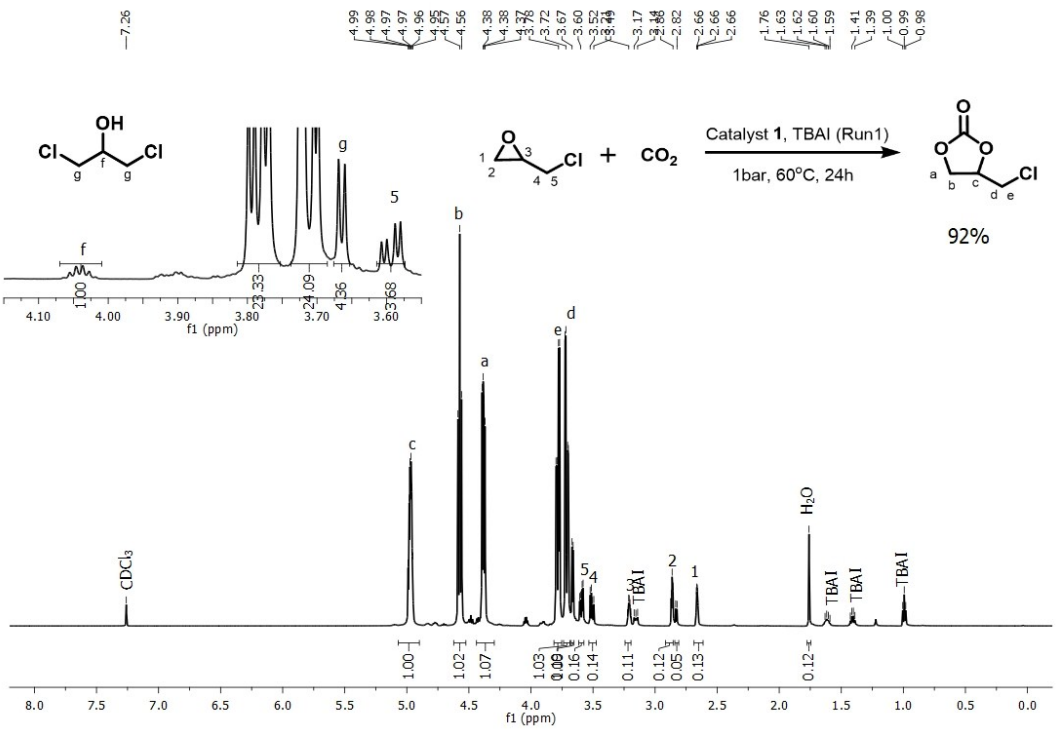


Figure S19. Crude ^{1}H-NMR spectra of cycloaddition of CO_2 to Epichlorohydrin by using catalyst **1** with TBAI (Run 1, Table 3, Entry 5).

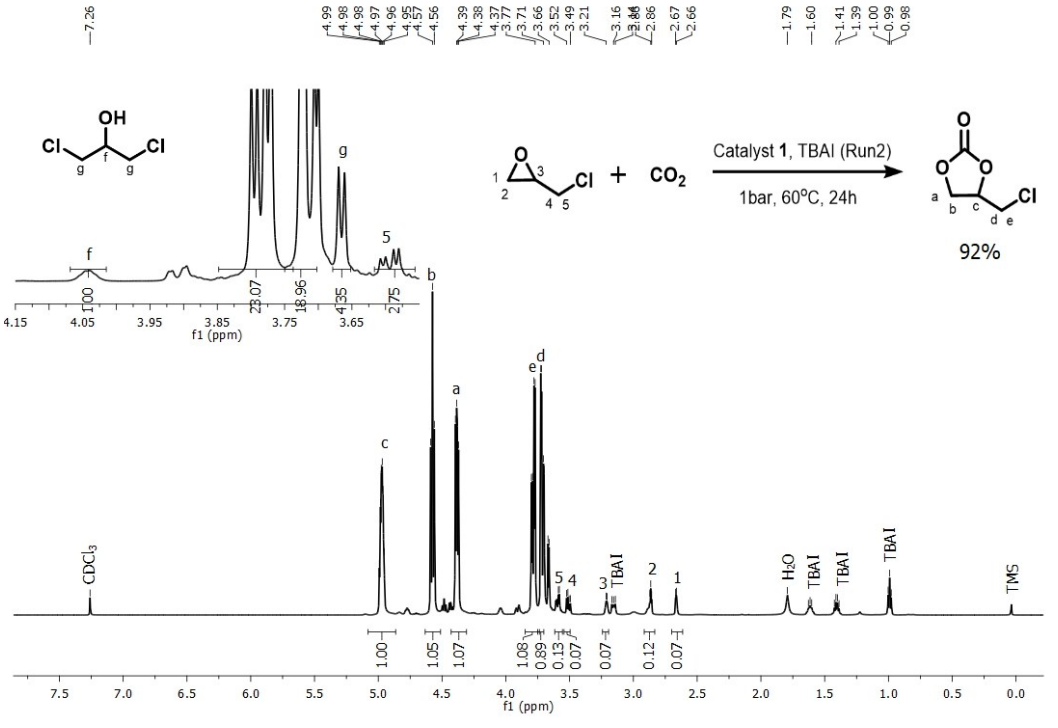


Figure S20. Crude ^{1}H-NMR spectra of cycloaddition of CO_2 to Epichlorohydrin by using catalyst **1** with TBAI (Run 2, Table 3, Entry 5).

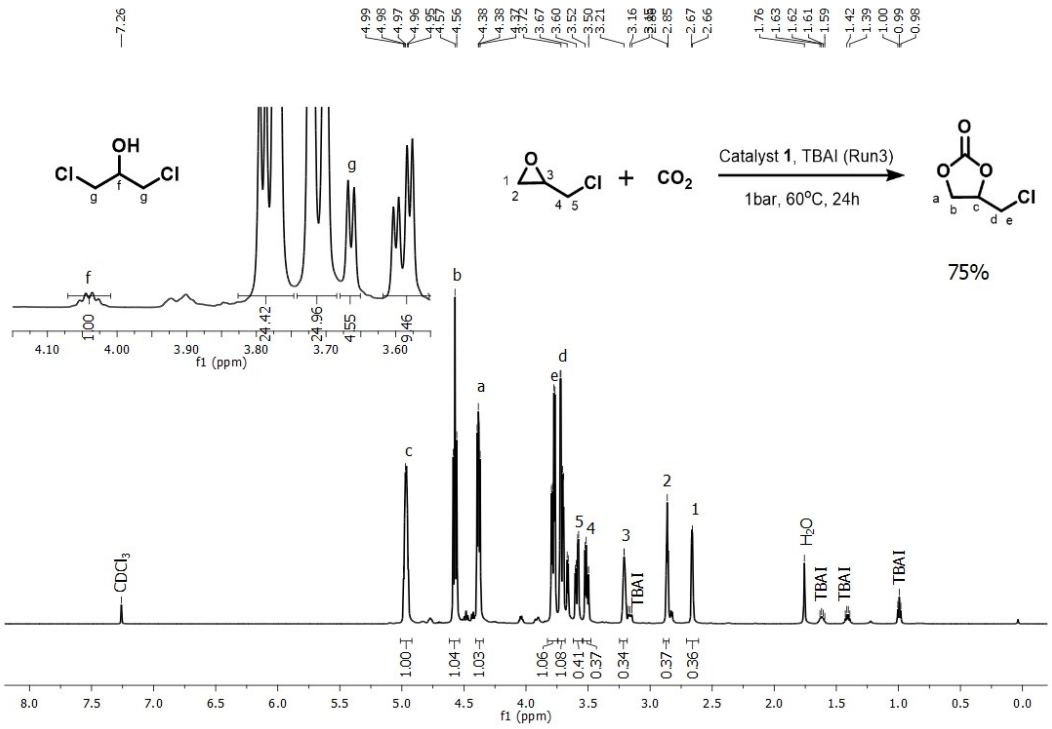


Figure S21. Crude ^{1}H-NMR spectra of cycloaddition of CO_2 to Epichlorohydrin by using catalyst **1** with TBAI (Run 3, Table 3, Entry 5).

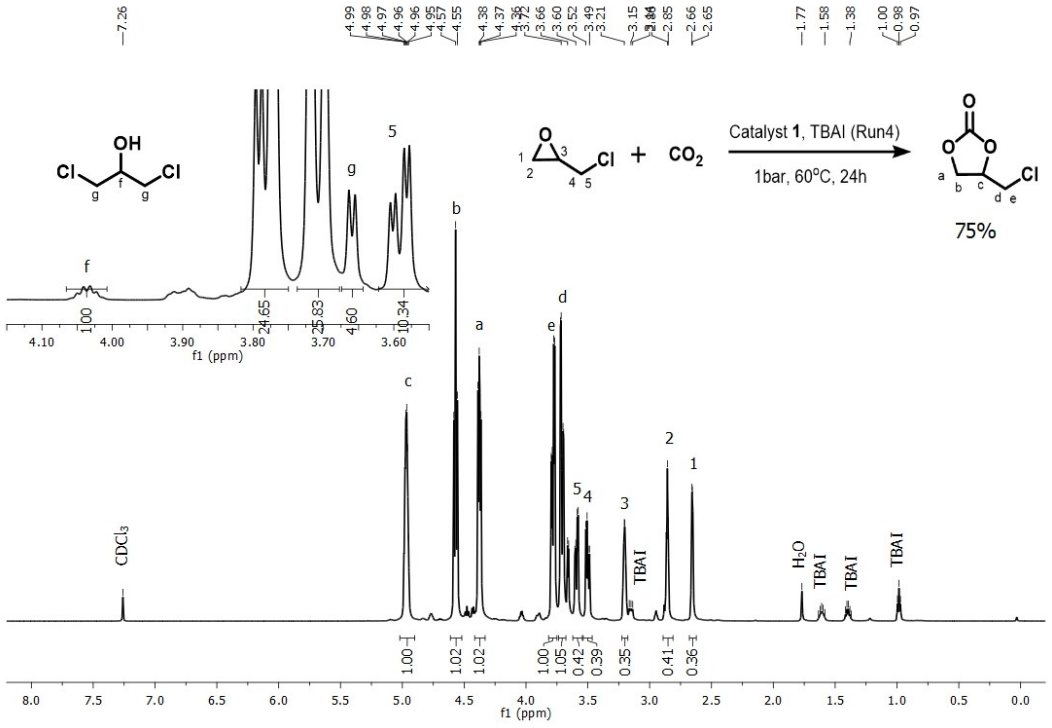


Figure S22. Crude ^{1}H-NMR spectra of cycloaddition of CO_2 to Epichlorohydrin by using catalyst **1** with TBAI (Run 4, Table 3, Entry 5).

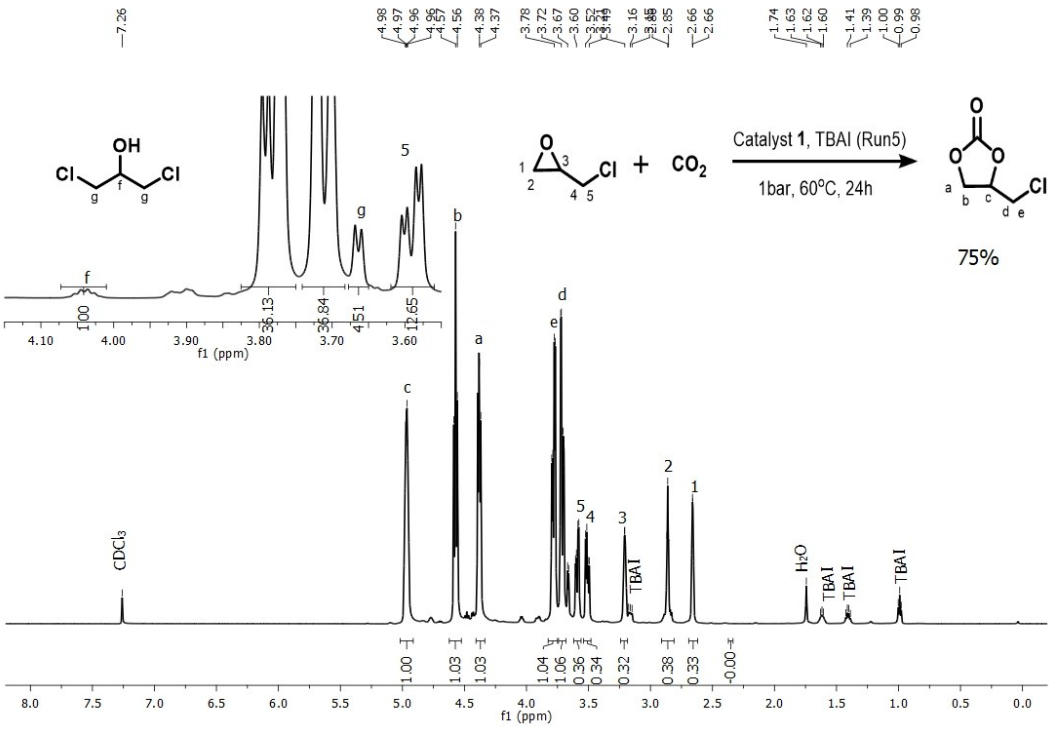


Figure S23. Crude ^{1}H-NMR spectra of cycloaddition of CO_2 to Epichlorohydrin by using catalyst **1** with TBAI (Run 5, Table 3, Entry 5).

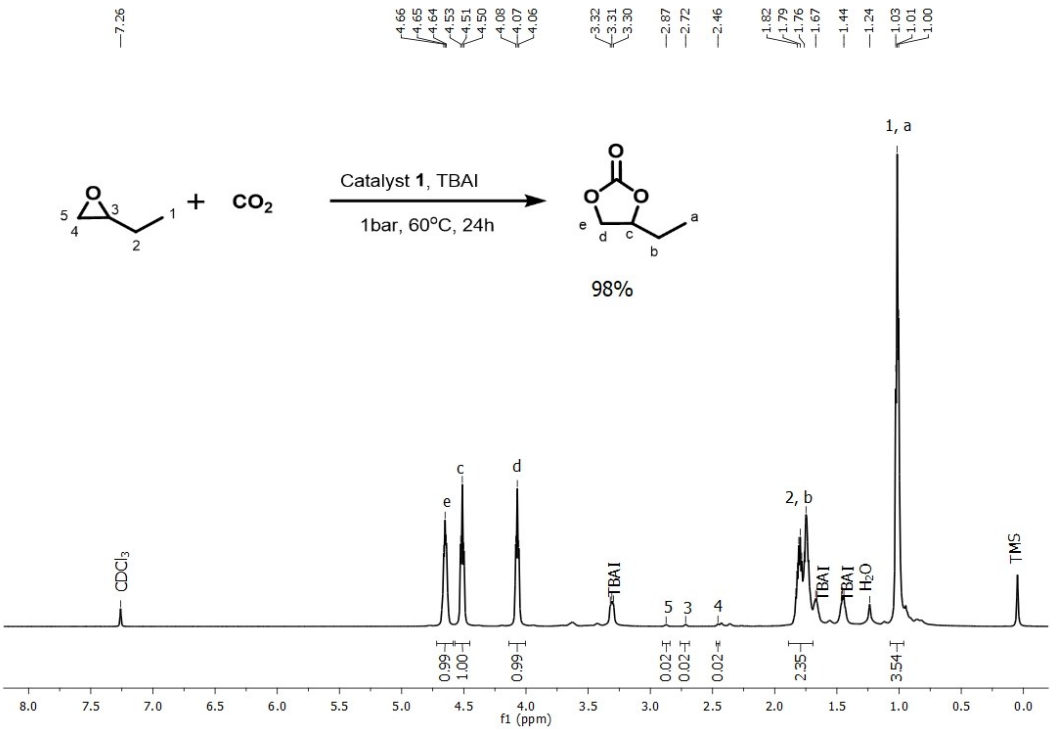


Figure S24. Crude ^{1}H-NMR spectra of cycloaddition of CO_2 to epoxybutane by using catalyst **1** with TBAI (Table 3, Entry 6).

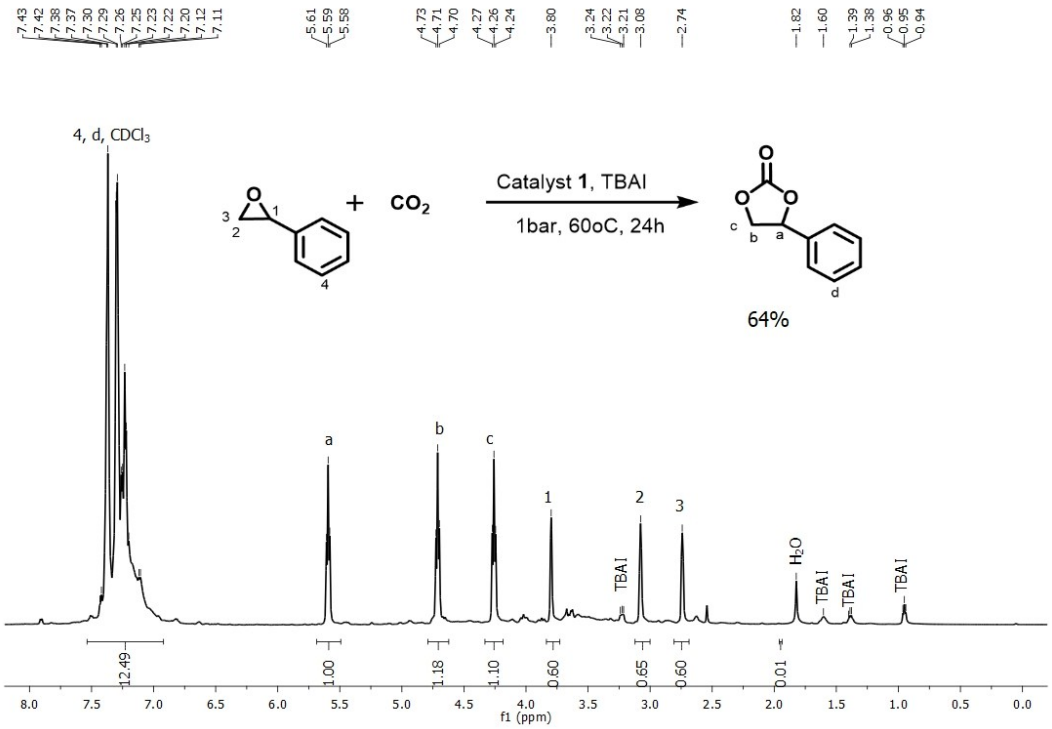


Figure S25. Crude ^{1}H-NMR spectra of cycloaddition of CO_2 to Styrene oxide by using catalyst **1** with TBAI (Table 3, Entry 7).

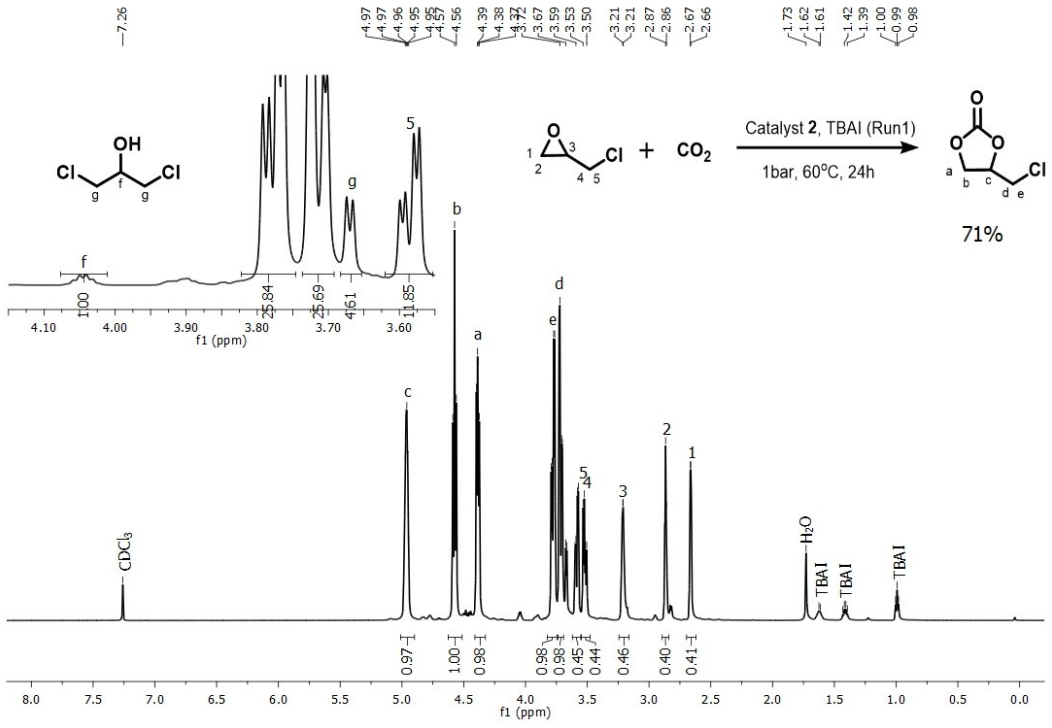


Figure S26. Crude ^{1}H-NMR spectra of cycloaddition of CO_2 to Epichlorohydrin by using catalyst **2** with TBAI (Run 1, Table 3, Entry 8).

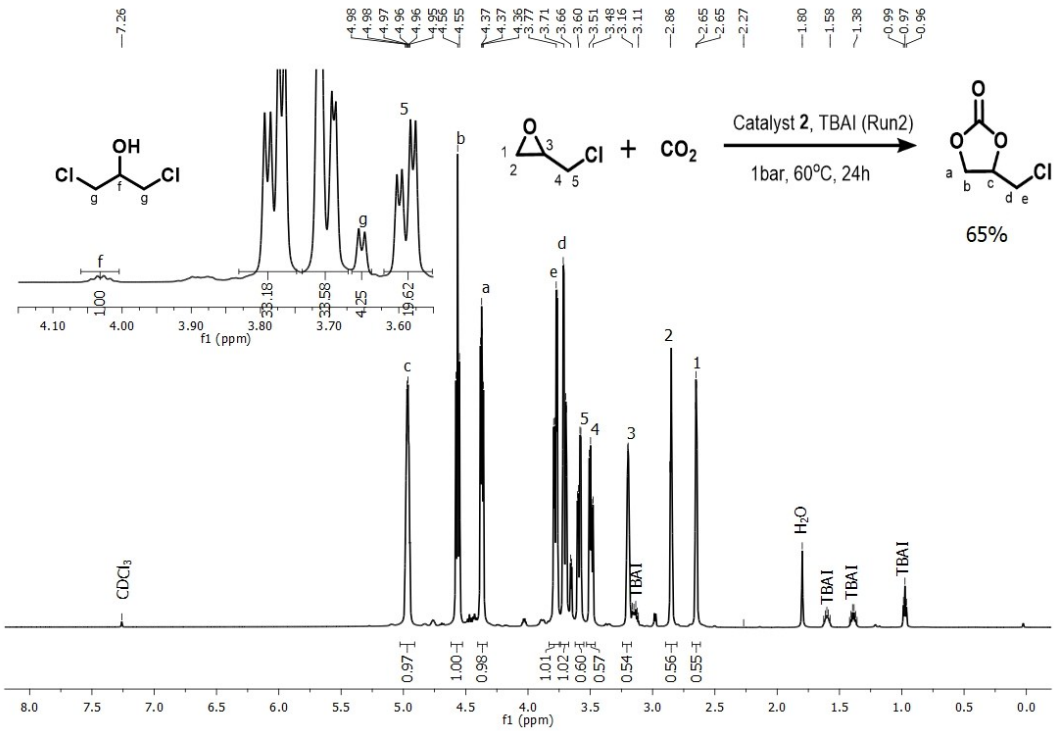


Figure S27. Crude ^{1}H-NMR spectra of cycloaddition of CO_2 to Epichlorohydrin by using catalyst **2** with TBAI (Run 2, Table 3, Entry 8).

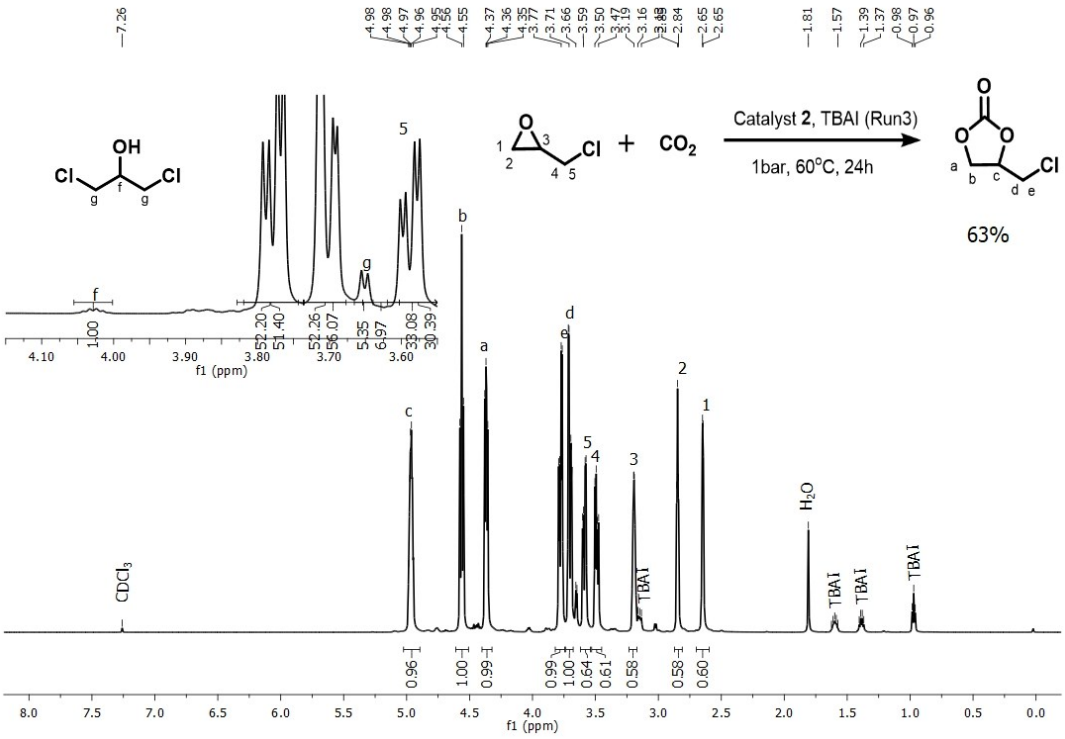


Figure S28. Crude ^{1}H-NMR spectra of cycloaddition of CO_2 to Epichlorohydrin by using catalyst **2** with TBAI (Run 3, Table 3, Entry 8).

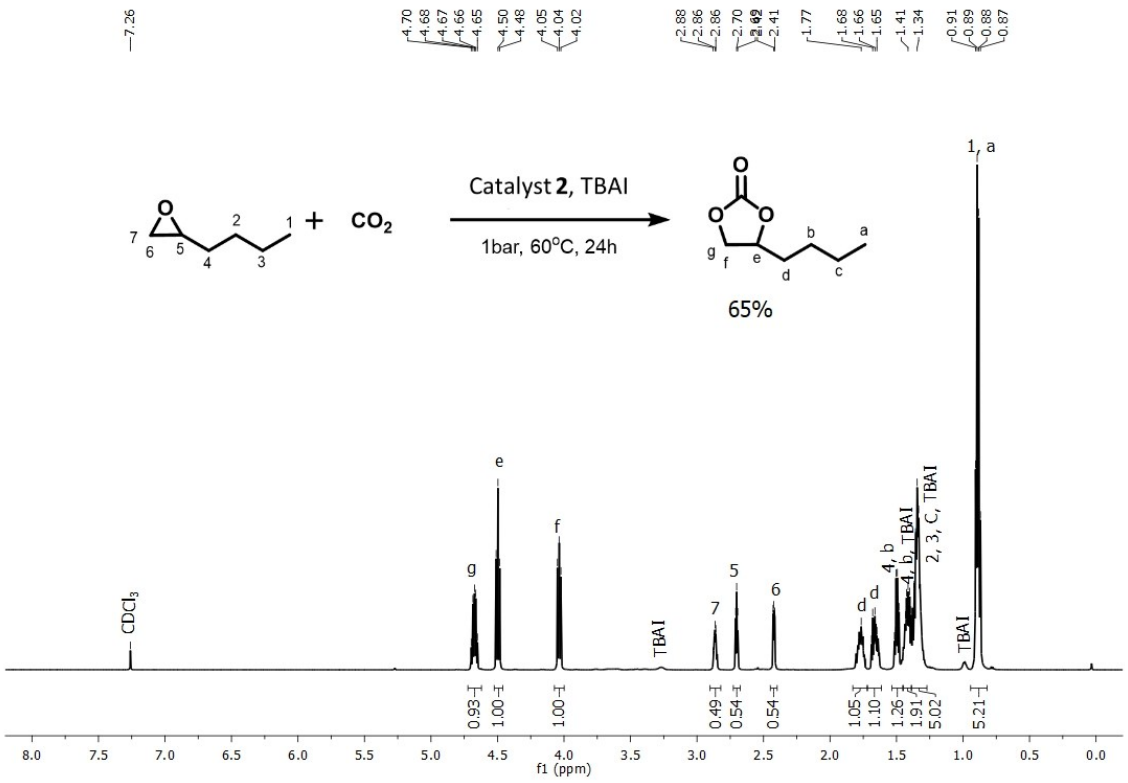


Figure S29. Crude ^{1}H-NMR spectra of cycloaddition of CO_2 to 1,2-Epoxyhexane by using catalyst **2** with TBAI (Table 3, Entry 9).

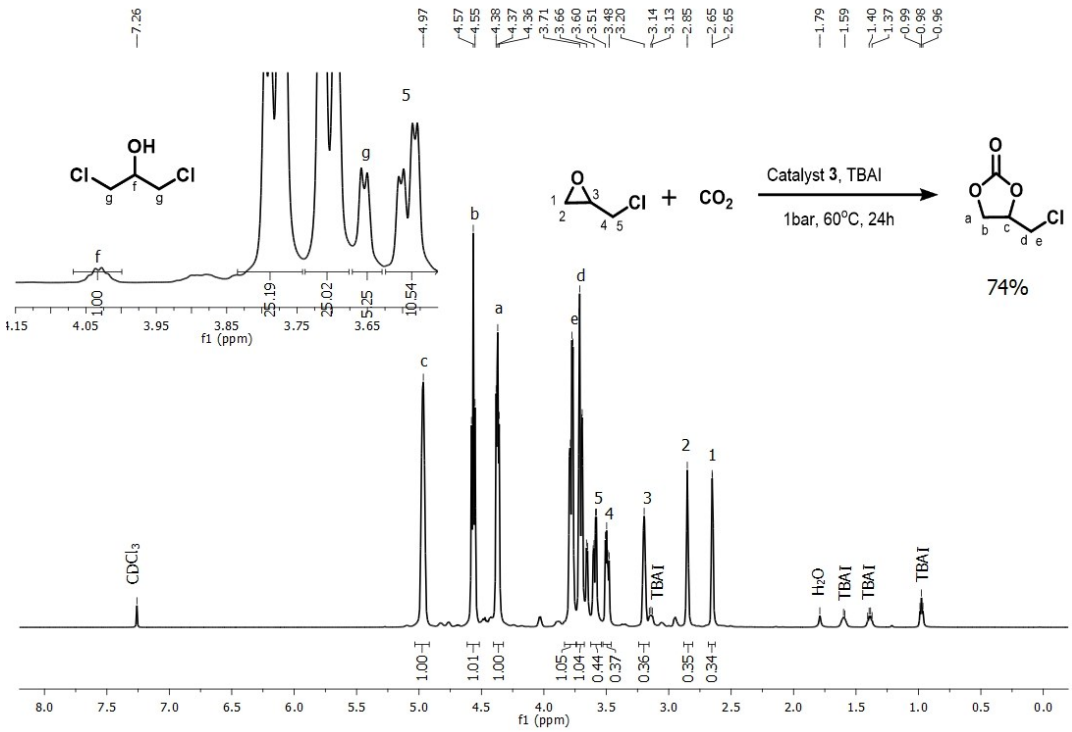


Figure S30. Crude ^{1}H-NMR spectra of cycloaddition of CO_2 to Epichlorohydrin by using catalyst **3** with TBAI (Table 3, Entry 10).

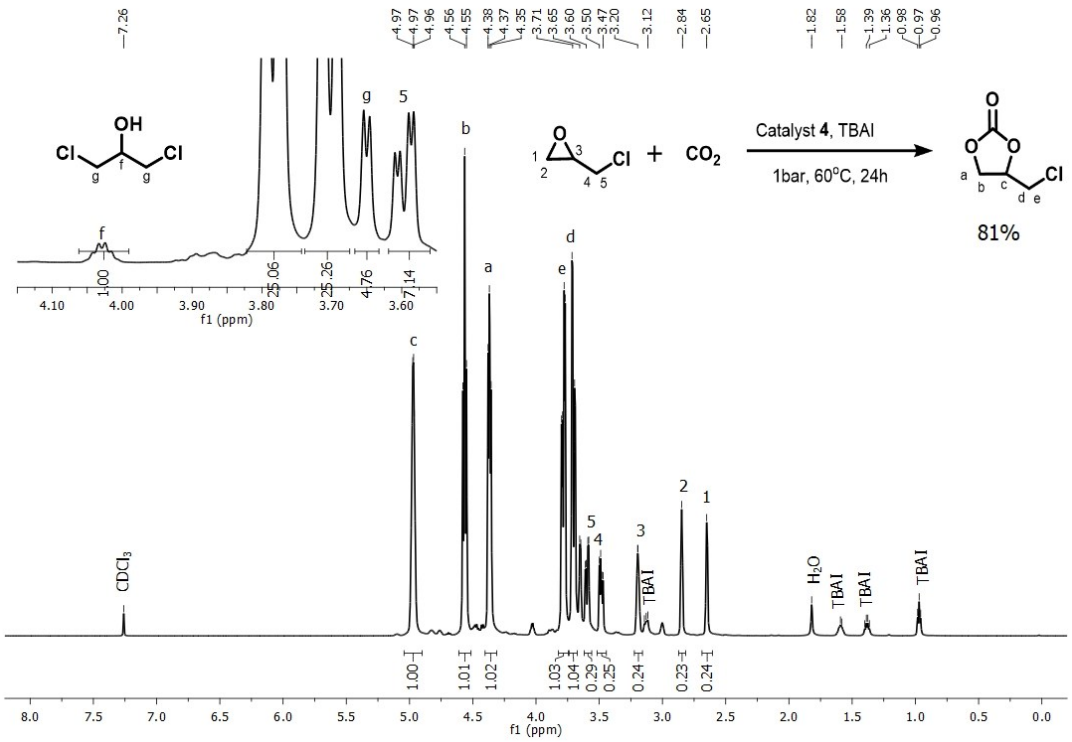


Figure S31. Crude ^{1}H-NMR spectra of cycloaddition of CO_2 to Epichlorohydrin by using catalyst **4** with TBAI (Table 3, Entry 11).

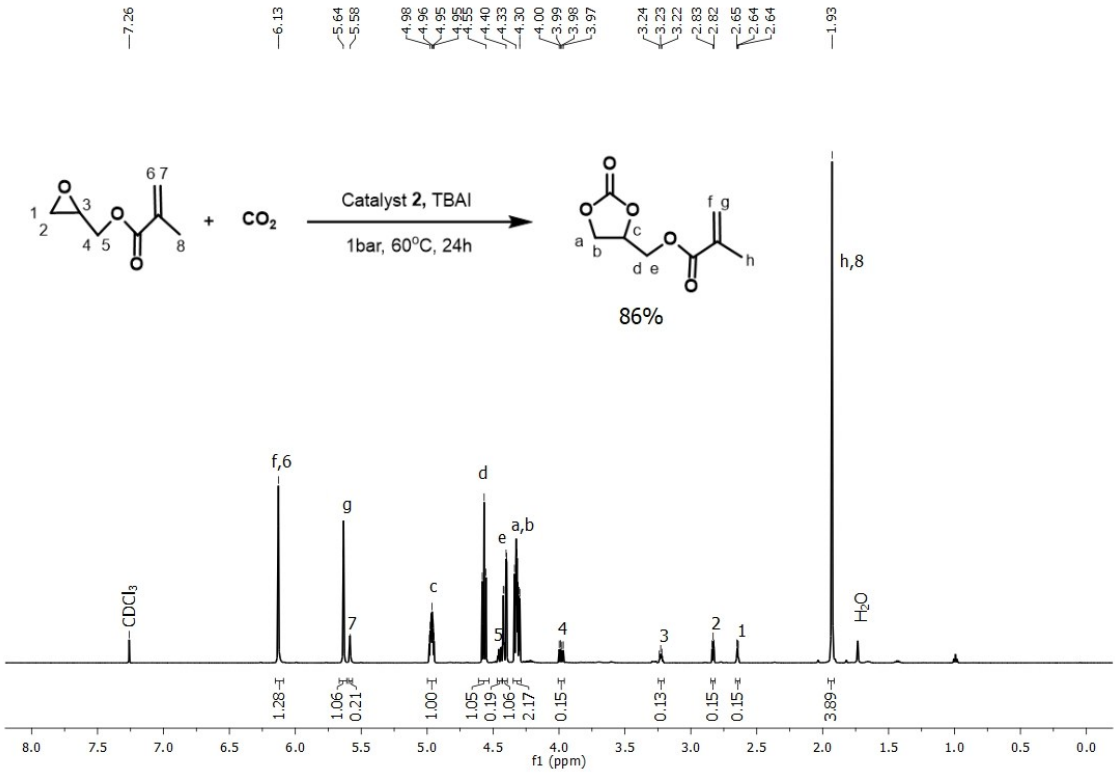


Figure S32. Crude ^{1}H-NMR spectra of cycloaddition of CO_2 to Glycidyl methacrylate (**5f**) by using catalyst **2** with TBAI at 60°C for 24 h (Table 3, Entry 12).

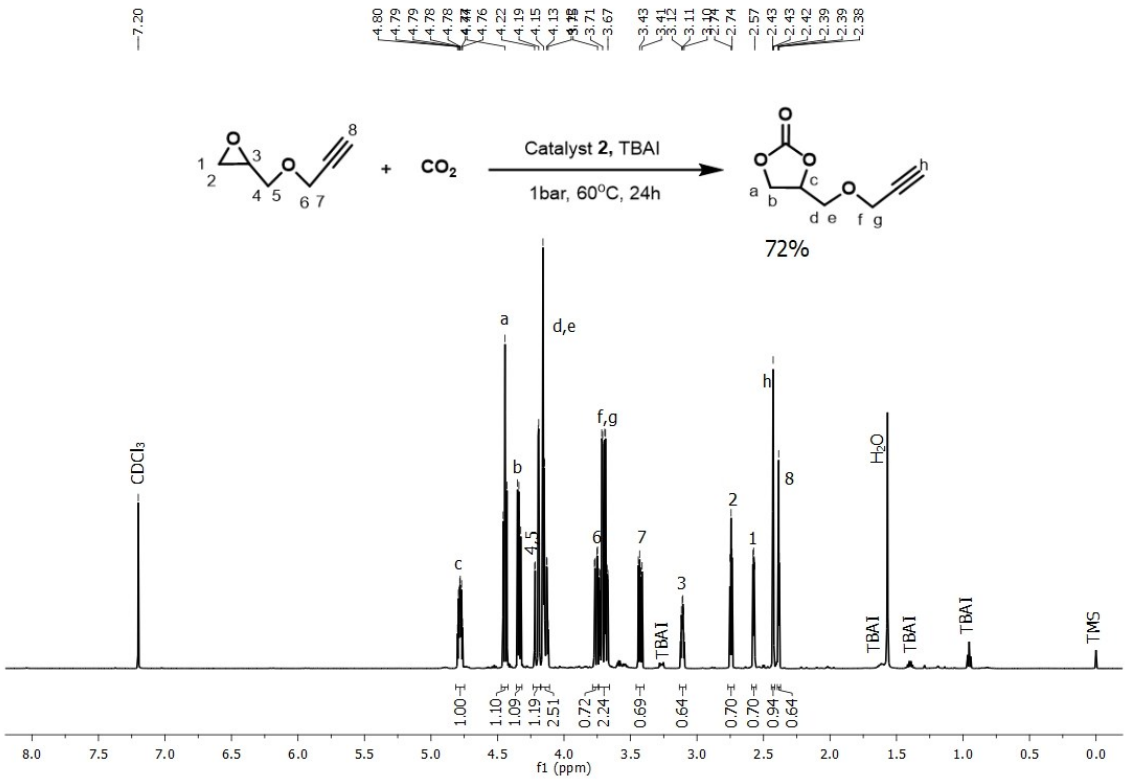


Figure S33. Crude ^{1}H-NMR spectra of cycloaddition of CO_2 to glycidyl propargyl ether (**5g**) by using catalyst **2** with TBAI at 60°C for 24 h (Table 3, Entry 13).

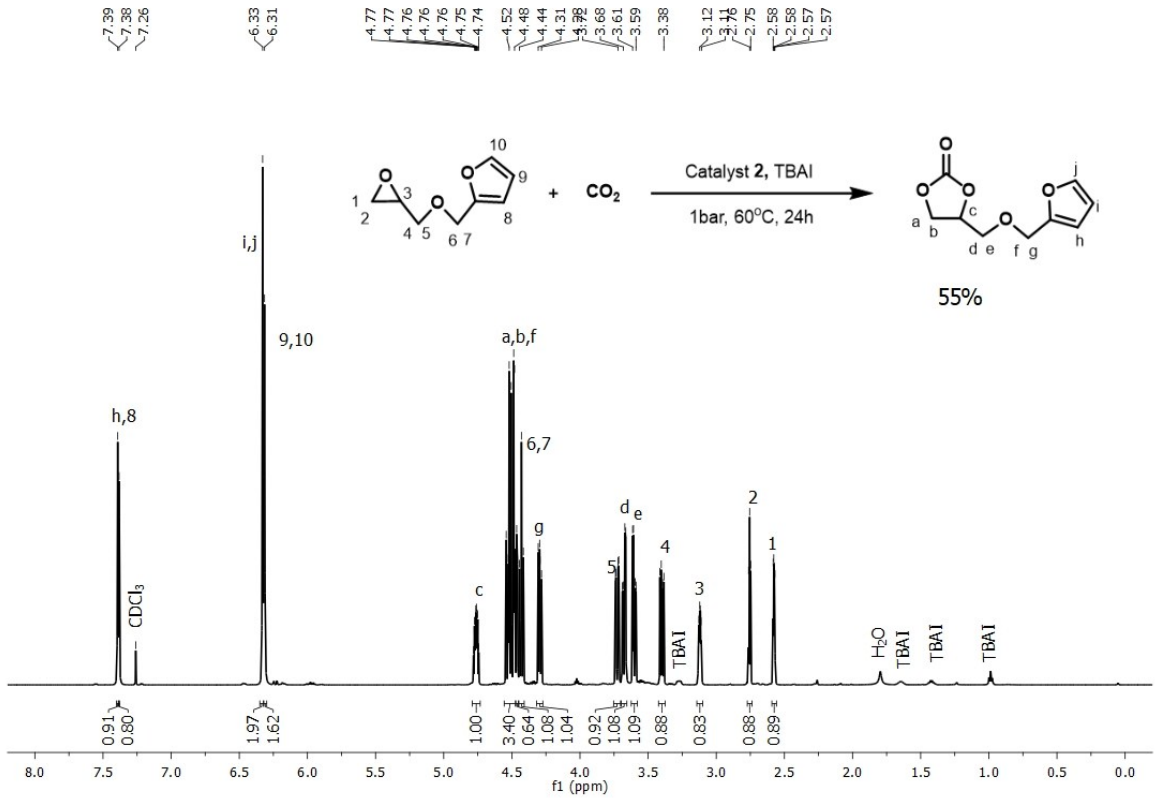


Figure S34. Crude ^{1}H-NMR spectra of cycloaddition of CO_2 to furfuryl glycidyl ether (**5h**) by using catalyst **2** with TBAI at 60°C for 24 h (Table 3, Entry 14).

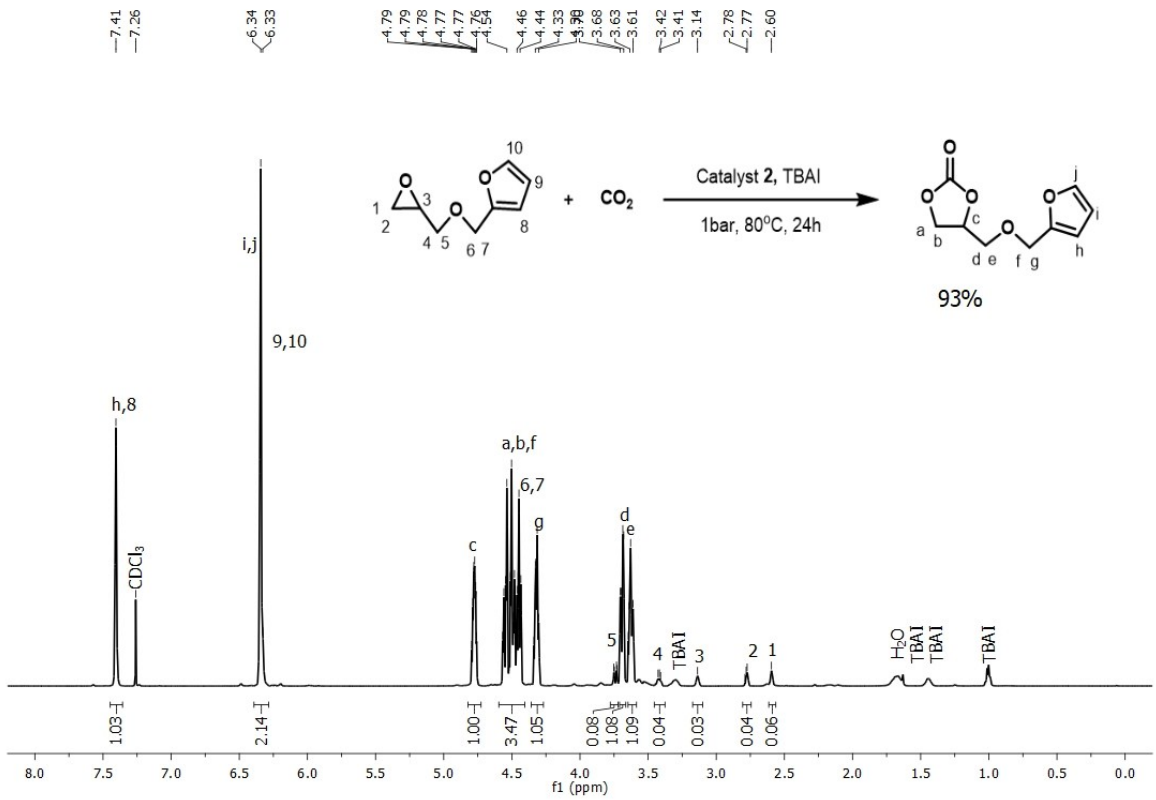


Figure S35. Crude ^{1}H-NMR spectrum of cycloaddition of CO_2 to furfuryl glycidyl ether (**5h**) by using catalyst **2** with TBAI at 80°C for 24 h (Table 3, Entry 15).

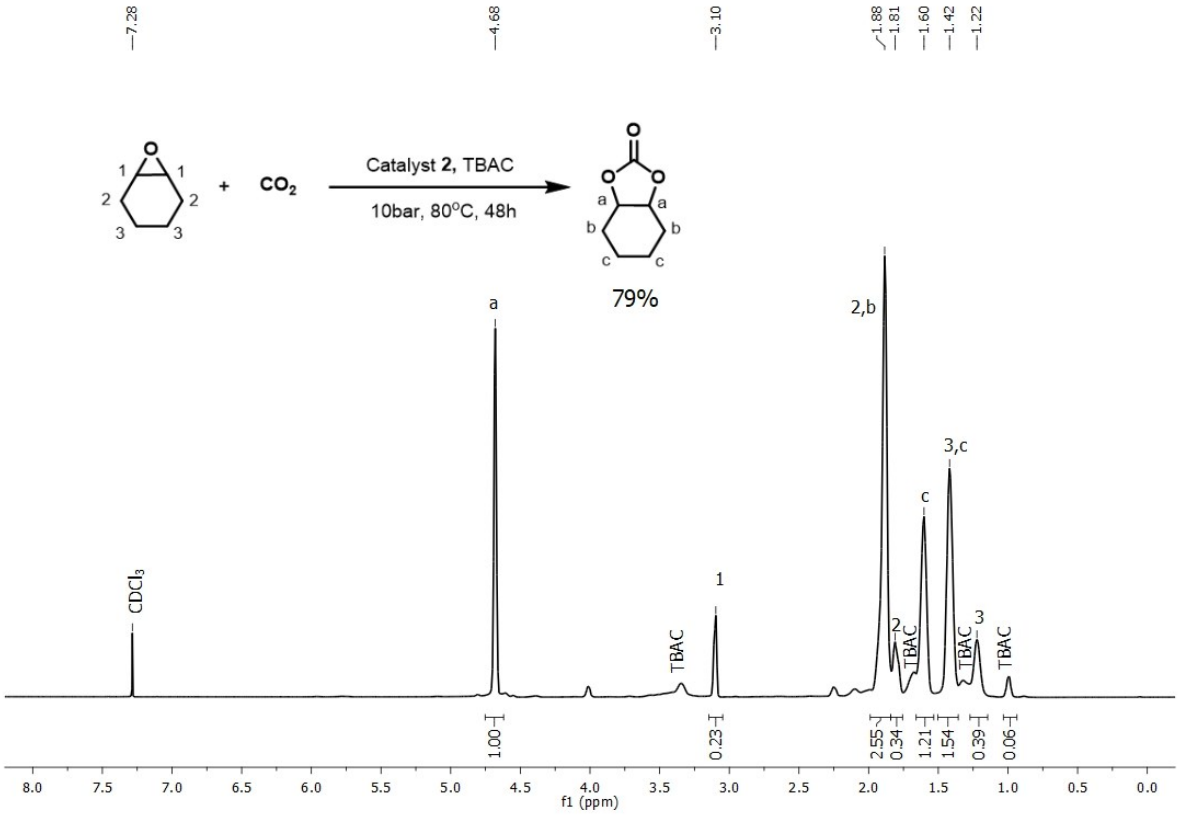


Figure S36. Crude ^{1}H-NMR spectrum of cycloaddition of CO_2 to cyclohexene oxide (**5i**) by using catalyst **2** with TBAC at 80°C, 10 bar CO_2 for 48 h (Table 3, Entry 16).

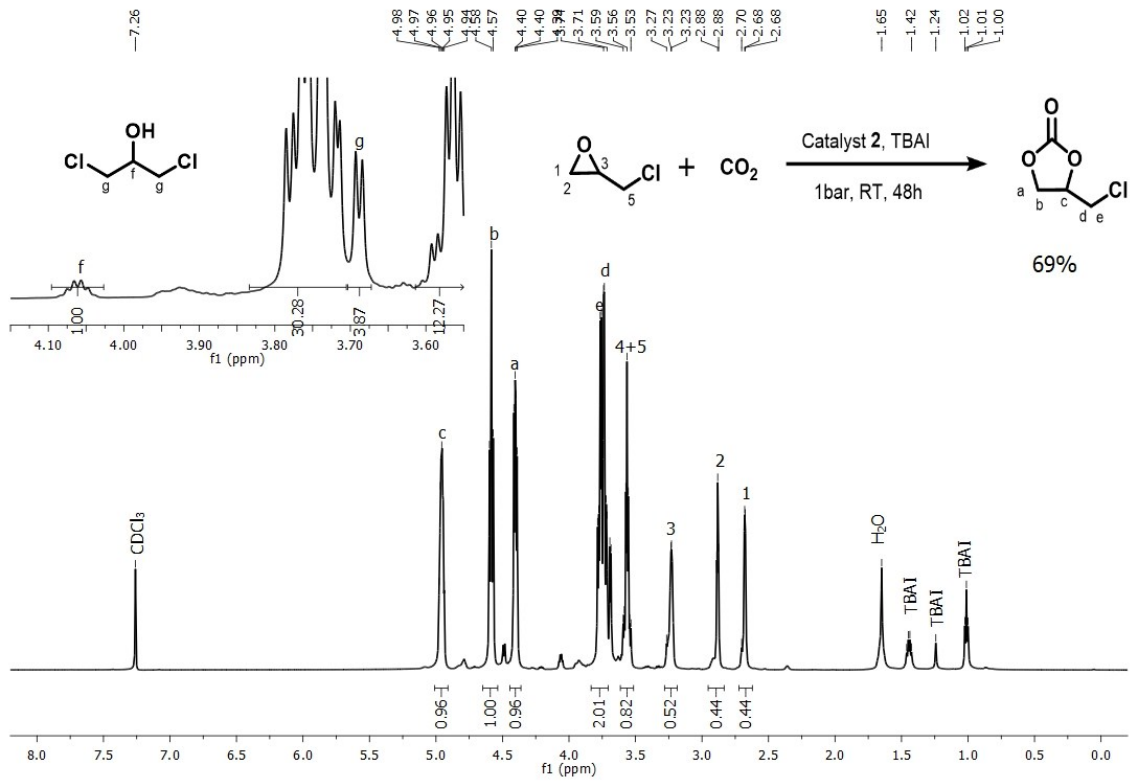


Figure S37. Crude ^{1}H-NMR spectra of cycloaddition of CO_2 to Epichlorohydrin by using catalyst **2** with TBAI at room temperature for 48 h (Table 3, Entry 18).

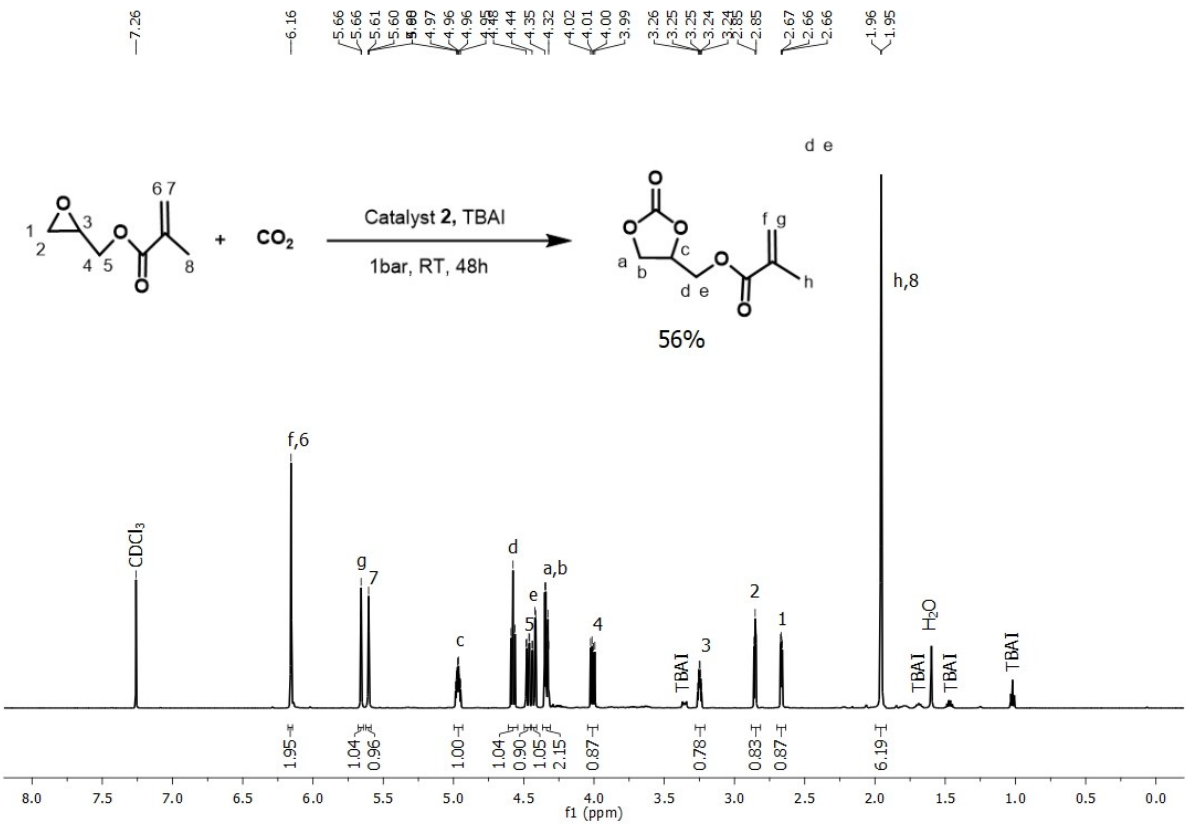


Figure S38. Crude ^{1}H-NMR spectrum of cycloaddition of CO_2 to glycidyl methacrylate (**5h**) by using catalyst **2** with TBAI at room temperature for 48 h (Table 3, Entry 19).

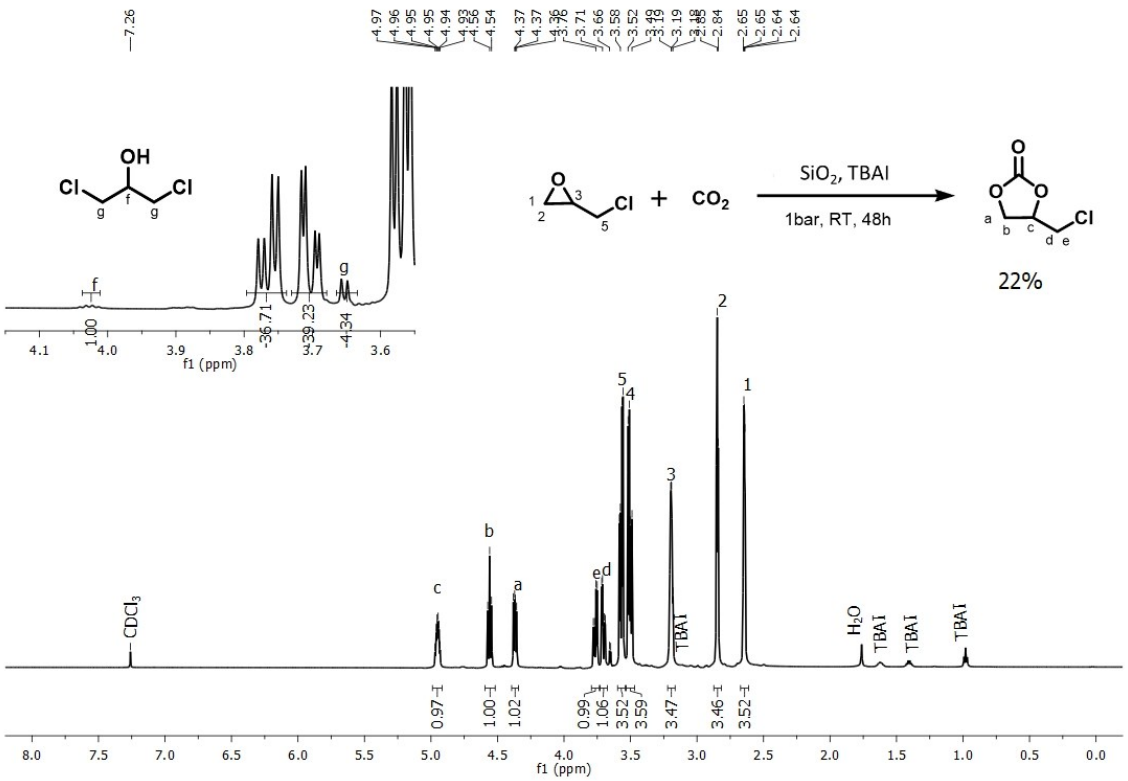


Figure S39. Crude ^{1}H-NMR spectra of cycloaddition of CO_2 to Epichlorohydrin by using tt-SiO_2 with TBAI at room temperature for 48 h (Table 3, Entry 20).

Table S3. Comparison of Lewis acids for the cycloaddition of CO_2 to propylene oxide under ambient conditions.

Entry	Catalyst	Loading (mol%) Lewis acid/TBAX)[a]	TBAX/Lewis acid (molar ratio)	Conv. (%)	C atoms/metal (molar ratio)	Time (h)	TON/ TOF(h^{-1})	Ref.
1	**2**/TBAI	0.5/1	2	73	3	48	146/ 3.0	This work
2	$ZrCl_2(O_2CNEt_2)_2$@SiO_2 /TBAB	0.5/1	2	40 (63)[b]	8	24	50[c]	7
3	Zn-Al/LDH-RM[d]/TBAB	1.65[e]/3.6	2.2	74	4	24	44.8	8
4	In-MOF/TBAB	0.46/5	10.9	78	10.2	48	170	9
5	Hf-NU-1000/TBAB	4/10	2.5	100	14.7	26	25	10
6	MMPF-18/TBAB (Zn-porphyrin MOF)	0.25[f]/7.2	28.8	97	34	48	388	11
7	MMCF-2/TBAB (Cu-MOF)	0.125/7.2	57.6	95	15	48	763	12
8	Zn/Tb heterometallic helicate/TBAB	0.875[g]/7.2	8.2	96	10.2	48	109	13
9	Al(III)-Salen cage/TBAB	1[h]/10	10	58	32	48	58	14
10	Single Component Al(III) bimetallic salen on Merrifield resin	2.5	1[i]	100[j]	33	20	40	15
11	Co(III)-Salen conjugated microporous polymer/TBAB	0.49/7.2	14.7	81.5	40	48	167	16

[a] X = Br or I.

[b] The value in brackets denotes the selectivity for **6b**.

[c] TON and TOF values relative to the cyclic carbonate product.

[d] Layered double hydroxide (LDH) prepared by reverse micelle (RM) method with the formula $[Zn_2Al(OH)_6](C_{12}H_{25}SO_4)\cdot 0.6H_2O]$ according to reference [17]

[e] Refers to the combined loading of aluminum and zinc atoms calculated from the approximated formula $[Zn_2Al(OH)_6](C_{12}H_{25}SO_4)$ (Al: 5.14 %; Zn: 24.9 %) and based on the use of 34.5 mmol of **5b** in the presence of 100 mg Zn-Al/LDH-RM (Al: 5.14 mg, 0.19 mmol, 0.55 mol%; Zn: 24.9 mg, 0.38 mmol; 1.1 mol%. Total Lewis acid loading (Al+Zn) =1.65 mol%) as reported in reference [8].

[f] Refers only to the Zn loading in the porphyrin ring but not to Zn atoms in the MOF nodes.

[g] Considering the use of 0.125 mol% heterometallic helicate corresponding to (based on the formula $Zn_4Tb_3C_{72}H_{79}N_{18}O_{53}$) 0.5 mol% Zn and 0.375 Tb. Total Lewis acid loading (Zn+Tb): 0.875 mol%.

[h] Based on Al(III)-Salen cage loading 0.33 mol% corresponding approximatively to 1 mol% Al.

[I] Quaternary ammonium unit included in the single-component catalyst. [j] Using **5e** as the substrate.

S7: *Kinetic data for CO_2 reaction order*

Kinetic data were collected by *in situ* IR in the form of apparent initial reaction rates (k_{obs}; Table S4) as described above in section S1. The data were collected from the reaction of CO_2 cycloaddition to epichlorohydrin (2 mL, 25.5 mmol) at room temperature using YCl_3 (50 mg, 1 mol%) and tetrabutylammonium iodide (TBAI, 188.4 mg, 2 mol%) as homogeneous catalyst (Table S4, Entries 1-5) or compound **2** (370 mg, 1 mol% Y) and TBAI (188.4 mg, 2 mol%) as catalytic system (Table S4, Entry 6). The logarithmic plot in Figure S40 was obtained by plotting $\ln(k_{obs})$ versus $\ln(P_{CO2})$ for the homogeneous YCl_3/TBAI system. It is possible to use $\ln(P_{CO2})$ in place of $\ln([CO_2])$, being $[CO_2]$ the concentration of CO_2 in the epoxide solution, because it was previously shown that $[CO_2]$ in epoxide varies linearly with P_{CO2} in the 1-10 bar range.[18] A fractional reaction order in CO_2 (0.47) was obtained.

Table S4. Measured apparent initial reaction rates (k_{obs}) for reactions catalyzed by YCl_3/TBAI (Entries 1-5) and **2**/TBAI (Entry 10).

Entry	P_{CO2} (bar)	$\ln(P_{CO2})$	k_{obs} (a.u.)	$\ln(k_{obs})$
1	2	0.69	0.0637	-1.19
2	4	1.39	0.0745	-1.13
3	6	1.79	0.0863	-1.06
4	8	2.08	0.1213	-0.92
5	10	2.3	0.132	-0.88
6	10		0.027	

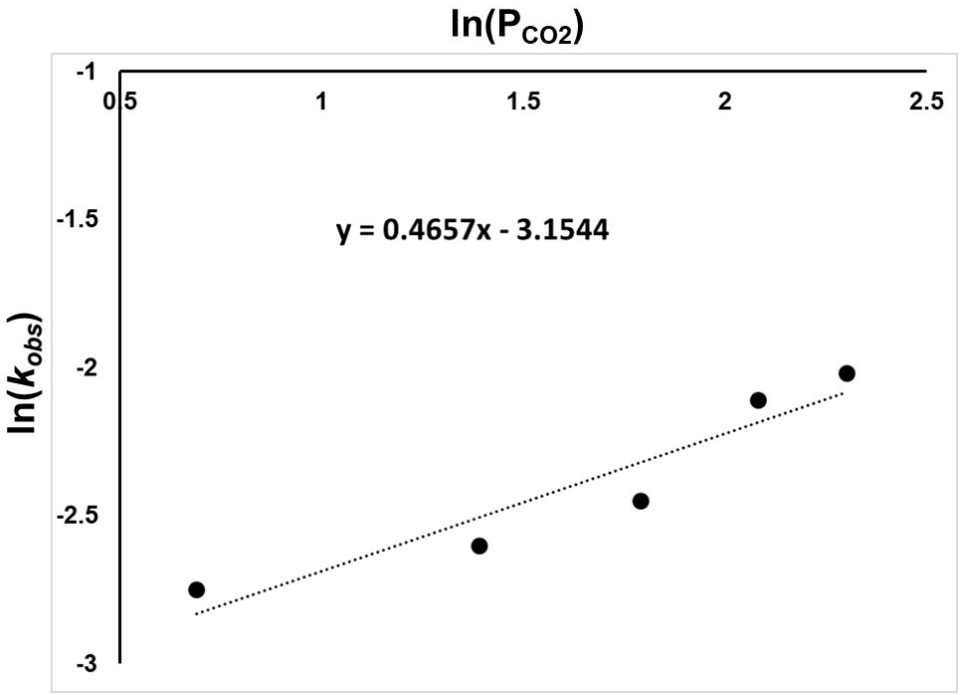


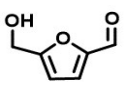
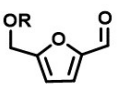
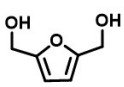
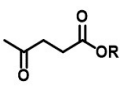
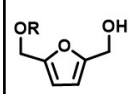
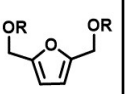
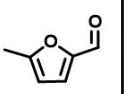
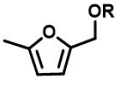
Figure S40. Logarithmic plot of apparent reaction rates (k_{obs}) at different CO_2 pressures for the cycloaddition of CO_2 to epichlorohydrin catalyzed by homogeneous YCl_3/TBAI.

S8: *Supporting data for HMF reductive etherification*

Standard reaction procedure: A typical reaction was carried out in a 50 mL stainless steel autoclave containing isopropanol (10 mL), material **2** (50.3 mg, 0.03 mmol Y, 4.8 mol%) and 5-hydroxymethyl furfural (HMF; 78.5 mg, 0.62 mmol). N_2 (20 bar) was added and the reactor was heated up to 150 °C and kept at this temperature for one to five hours.

Product analysis: The products were identified with a gas chromatograph-mass spectrometer (GC-MS) system (PerkinElmer GC Clarus 680 with MS clarus SQ 8T) equipped with Elite-5 MS column. HMF conversion were determined by mean of a calibration curve built using HMF solutions of different concentration in 10 mL isopropanol. Octane (5 µL for 1 mL of standard solution) was added as internal standard. At the end of each reaction, the crude was concentrated under reduced pressure and the volume of the sample was readjusted to 10 mL by adding the suitable amount of isopropanol followed by the addition of 5 µL octane to 1 mL aliquot of solution.

Table S5. Overview of catalytic reactions and products distribution in the reductive etherification of HMF by supported and homogeneous yttrium catalysts.[a]

Entry	Catalyst	HMF Conversion (%)	Product (%Yield)						
									
		HMF	**9**	**8a**	**10**	**8b**	**8c**	**11**	**11a**
		MW 126	MW 168	MW 128	MW 158	MW 170	MW 212	MW 110	MW 154
		9.79[b]	10.61	9.33	6.86	10.96	12.46	4.80	5.48
1	Blank	5.0	5.0						
2	$YCl_3 \cdot 6H_2O$[c]	75.0	4.0	3.0	5.0	7.0	35.0	15.0	6.0
3	YCl_3	90.4	1.5	0.13	2.0	15.0	71.2	0.42	0.05
4	**2**	90.0	1.45	24.4	0.80	54.8	8.3	0.18	
5[d]	**2**	92.6	0.47	20.0	3.0	55.9	12.5	0.68	0.11

[a] Reaction conditions:150°C, 1 h, 20 bar N_2. R represents isopropyl group.
[b] The entries in this row denote retention time in the gas chromatogram (min).
[c] Taken from reference [19].
[d] Reaction time: 5 h.

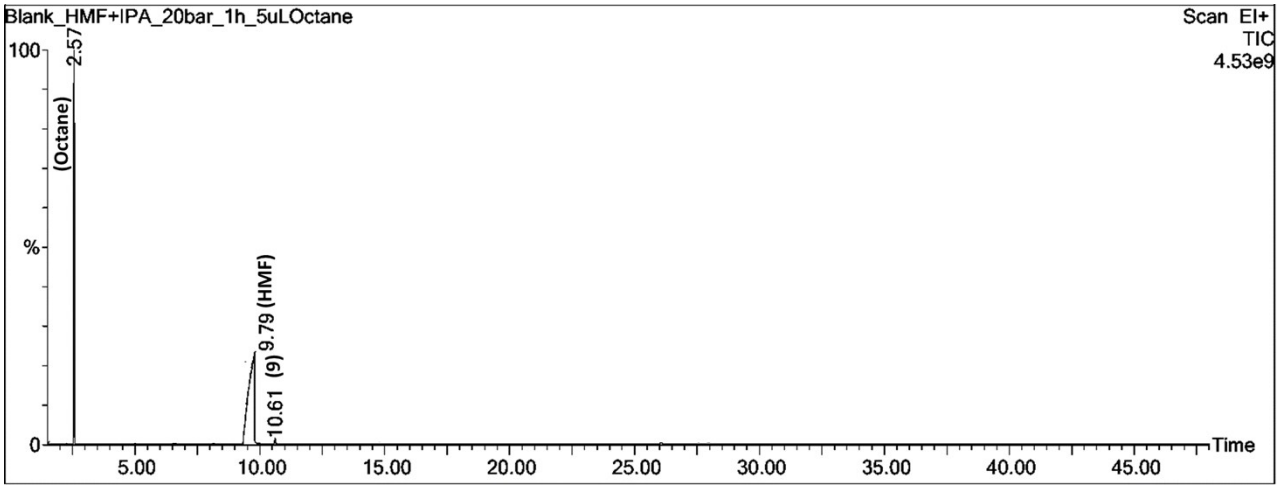


Figure S41. Chromatogram of reductive etherification of HMF without catalyst (blank reaction) at 150 °C, 20 bar N_2 for 1 h (Table S5, Entry 1).

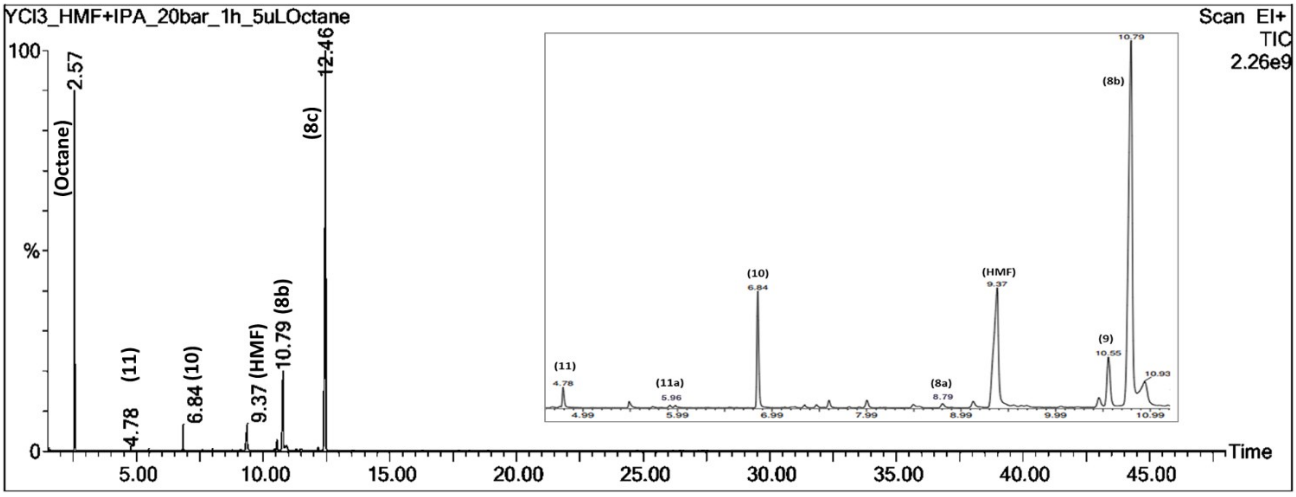


Figure S42. Chromatogram of reductive etherification of HMF catalyzed by YCl_3 at 150 °C, 20 bar N_2 for 1 h (Table S5, Entry 3).

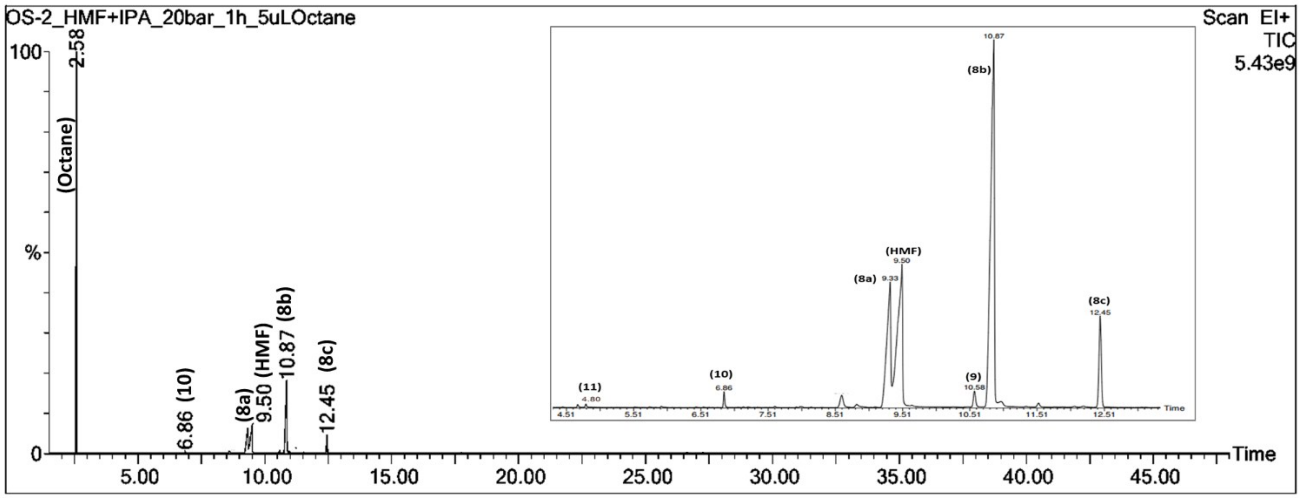


Figure S43. Chromatogram of reductive etherification of HMF catalyzed by **2** at 150 °C, 20 bar N_2 for 1 h (Table S5, Entry 4).

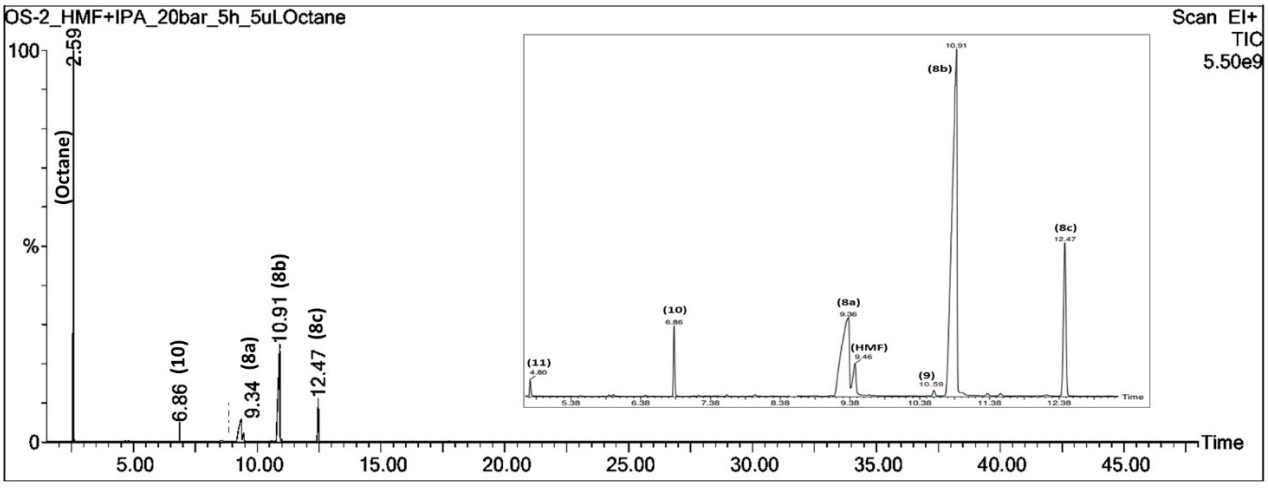
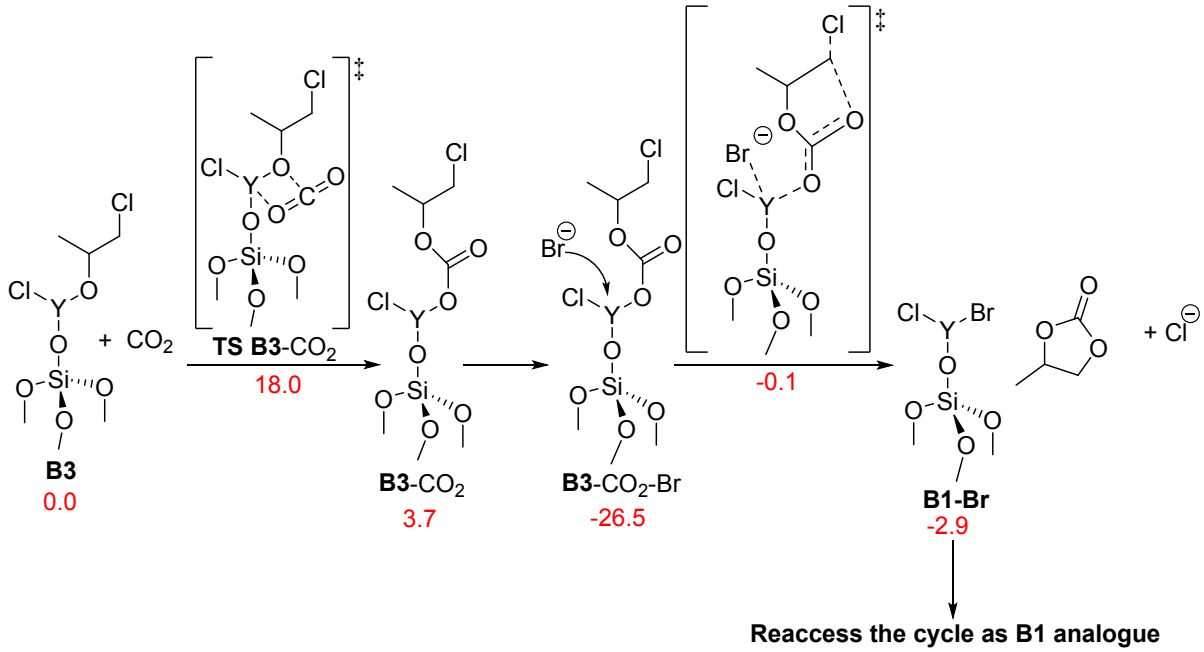


Figure S44. Chromatogram of reductive etherification of HMF catalyzed by **2** at 150 °C, 20 bar N_2 for 5 h (Table S5, Entry 5).

S9: *Supporting data of DFT calculations*



Scheme S1. Alternative mechanism for the formation of cyclic carbonate from **B3** with formation of **B1**-Br as surface complex. The values in red refer to calculated Gibbs free energies (kcal/mol) of intermediates and transition states (in square brackets) relative to **B3**.

All the DFT geometry optimizations were performed at the GGA BP86 level,[20-22] D3 version of Grimme's dispersion (empiricaldispersion=gd3bj),[23, 24] with the Gaussian09 package.[25] The electronic configuration of the systems was described with the SVP basis set for the main group atoms,[26] whereas, for yttrium (Y), bromine (Br) and iodine (I), we adopted the quasi-relativistic SDD effective core potential.[27, 28] The reported free energies were built through single point energy calculations on the BP86-d3bj/SVP~sdd geometries using the M06 functional.[29, 30] and the cc-pVTZ basis set.[31] Solvent effects were included with the PCM model using the model propylene oxide (PO) solvent.[32, 33] To these electronic energies in solvent, zero point energy and thermal corrections were included from the gas-phase frequency calculations at the BP86-d3bj/SVP~sdd level.

Table S6. Absolute energies (in a.u.) and xyz coordinates of all computed species.

YCl_3:	
Y	**Y-PO**
SCF Done: -1418.94873702 A.U.	SCF Done: -1611.98582325 A.U.
Y 1.986385 -0.705043 -0.088399	Y 1.590767 -0.217265 0.071613
Cl 0.492722 -1.653704 1.612889	Cl 1.298014 -1.332122 2.262950
Cl 4.118319 0.314330 0.577370	Cl 3.764280 0.770038 -0.612989
Cl 1.156267 -0.405019 -2.378796	O 0.462526 1.772166 0.144540
	C -0.834773 2.237811 -0.330819
As a dimer:	C 0.382685 2.615333 -1.078946
SCF Done: -2837.98822927 A.U.	H -1.482425 1.436018 -0.727013
Cl 1.299593 7.433352 2.751520	H 0.585770 2.018673 -1.989200
Y -0.428139 6.503689 1.295839	C 1.063327 3.946948 -0.975802
Cl -2.692245 7.383798 1.562755	H 2.161978 3.807424 -1.030845

Cl 0.348066 6.353066 -1.240979 Cl -0.348099 3.847940 1.240938 Y 0.428105 3.697316 -1.295881 Cl 2.692211 2.817205 -1.562798 Cl -1.299628 2.767654 -2.751561	H 0.755377 4.585209 -1.829684 H 0.809846 4.464312 -0.030015 H -1.302390 2.967796 0.351730 Cl 0.168593 -0.976961 -1.827595
$\mathbf{I}_{AB}$ (X = Br)	**B** (X = Br)
SCF Done: -1625.52879453 A.U. Br -2.374004 3.959103 1.105297 C -0.245044 1.728958 0.833159 C 0.687723 2.844629 0.815009 C -0.808398 1.100674 -0.403477 O 1.334254 1.521976 0.990893 Y 2.689023 0.186902 -0.140309 Cl 4.901611 0.214863 1.022737 Cl 1.560120 -2.044062 -0.165940 Cl 2.771039 1.278844 -2.386043 H 0.919053 3.329485 -0.149802 H 0.765138 3.486867 1.706370 H -0.210822 1.366196 -1.300040 H -1.833877 1.504184 -0.531005 H -0.856695 -0.003333 -0.303919 H -0.721131 1.500367 1.798782	SCF Done: -1625.56347810 A.U. Y 1.662906 -0.145782 -0.168801 Cl 0.732351 -0.697222 2.130954 Cl 4.117373 0.496981 0.013899 O 0.696900 1.536366 -0.836689 C -1.294609 2.850805 -0.576559 C 0.050005 2.662306 -1.283923 H -1.823422 3.773401 -0.885598 H -0.152086 2.597557 -2.386815 C 0.905897 3.923934 -1.028532 H 1.889995 3.787237 -1.520179 H 0.432546 4.848703 -1.423463 H 1.089334 4.042893 0.060310 H -1.168439 2.811692 0.522941 Cl 1.376498 -2.025148 -1.853263 Br -2.592744 1.344029 -0.987896
$\mathbf{I}_{BC}$ (X = Br)	**C** (X = Br)
SCF Done: -1814.03289603 A.U. Y 1.692026 -0.070814 0.130271 Cl 0.534871 -1.874033 1.492185 Cl 4.206398 0.125012 0.414894 O 0.808713 1.877241 -0.014483 C -1.301242 2.941338 -0.524884 C 0.116758 2.602008 -0.984977 H -1.883451 3.471921 -1.302719 H 0.042868 1.990616 -1.919492 C 0.860554 3.910453 -1.317985 H 1.883132 3.653983 -1.660961 H 0.353753 4.487930 -2.120475 H 0.948065 4.547203 -0.413425 H -1.298447 3.511223 0.422983 O 1.534982 1.417921 2.387133 C 0.997823 2.440765 2.094676 O 0.514938 3.517314 2.161888 Cl 1.320399 -0.629601 -2.314287 Br -2.361891 1.263273 -0.110257	SCF Done: -1814.03992652 A.U. Y -4.007876 3.544977 -1.291783 Cl -5.461694 5.613812 -1.148692 Cl -3.191471 3.516325 -3.683341 Cl -5.530100 1.643530 -0.625680 O -2.555096 4.336117 0.386679 C -0.530997 0.816814 1.236205 C 0.186628 2.154115 1.024913 H -1.016978 0.431167 0.325211 H 0.860884 2.321673 1.890277 C 0.983720 2.243742 -0.274790 H 1.765555 1.457982 -0.292582 H 0.315521 2.108012 -1.147212 H 1.478199 3.232759 -0.348489 H -1.252846 0.874408 2.071219 Br 0.807607 -0.616197 1.802884 C -1.815666 3.306829 0.299677 O -2.038057 2.363996 -0.524321 O -0.757578 3.249962 1.157419
$\mathbf{I}_{CD}$ (X = Br)	**D** (X = Br)
SCF Done: -1814.01805906 A.U. Y -4.398728 3.995605 -1.367749 Cl -5.433269 6.097598 -0.484941 Cl -3.266017 4.382951 -3.563495 Cl -6.079075 2.145771 -1.450893 O -2.818326 3.440658 0.053028 C -0.155038 0.779009 0.381240 C 0.244511 2.078664 1.070103 H 0.312901 0.466207 -0.556585 H 0.519168 1.879755 2.121704 C 1.345142 2.838655 0.342630 H 2.269561 2.228625 0.350690 H 1.051151 3.035252 -0.709491 H 1.542132 3.806361 0.844089 H -0.803889 0.060528 0.894260 Br 1.787856 -0.580685 1.453752 C -1.826233 2.655783 0.183070 O -1.605233 1.624015 -0.525912 O -0.947935 2.939018 1.158730	SCF Done: -1814.02802857 A.U. Y -4.480344 4.004110 -1.394351 Cl -5.480364 6.104052 -0.496507 Cl -3.342838 4.338945 -3.585269 Cl -6.119858 2.129794 -1.411833 O -2.833178 3.435524 -0.003865 C -0.402860 0.941952 0.189091 C 0.219984 2.076828 1.023345 H 0.239646 0.576181 -0.628832 H 0.444122 1.743473 2.052377 C 1.400800 2.781565 0.388719 H 2.242282 2.058195 0.393606 H 1.176790 3.087672 -0.655074 H 1.687642 3.676158 0.976026 H -0.757139 0.087367 0.793369 Br 2.027790 -0.588276 1.599966 C -1.828078 2.727119 0.218332 O -1.592834 1.600534 -0.425999 O -0.925399 3.047923 1.119452
$\mathbf{I}_{BC}$ (X = Br) dual	**C** (X = Br) dual
SCF Done: -3233.04028933 A.U. Y 2.876688 -1.475979 0.018118 Cl 1.697361 -0.574966 -2.065409 Cl 5.092499 -0.495147 0.749475 O 1.221013 -1.412928 1.346457 C 0.410278 0.796647 1.908709 C 0.712176 -0.631150 2.378055	SCF Done: -3233.08844262 A.U. Y 2.645308 -1.656969 -0.439911 Cl 3.654696 -0.186799 -2.198480 Cl 3.884231 -1.300945 1.747457 O 0.662996 -1.376959 1.051527 C 0.238565 0.886573 1.952003 C 0.528565 -0.573080 2.272893

H -0.006614 1.453197 2.693705 H 1.459481 -0.537380 3.209357 C -0.547218 -1.269318 2.993974 H -0.286644 -2.270681 3.390494 H -0.989216 -0.656372 3.804251 H -1.336969 -1.459371 2.231311 H -0.243794 0.809786 1.012954 Br 2.097549 1.679763 1.247502 Cl 3.320924 -3.932033 -0.321290 O -0.039709 -3.081083 -0.735353 C -0.507746 -2.038985 -0.520332 O -1.175030 -1.059090 -0.369343 Y -2.970143 0.032731 0.688845 Cl -3.975921 1.156862 -1.268207 Cl -2.951604 1.597163 2.629902 Cl -4.209448 -2.035375 1.259670	H 0.450285 1.515335 2.836853 H 1.559078 -0.658116 2.676415 C -0.470771 -1.187179 3.245431 H -0.177999 -2.233810 3.460923 H -0.452783 -0.623138 4.200094 H -1.511361 -1.189782 2.867657 H -0.789560 1.089371 1.595826 Br 1.464959 1.552951 0.489395 Cl 3.019465 -4.070816 -0.956073 O 0.332598 -1.666837 -1.091149 C -0.222569 -1.333232 -0.024440 O -1.418759 -0.981451 0.179656 Y -3.501744 -0.425540 0.489983 Cl -4.942158 -0.748789 -1.520884 Cl -3.247772 1.954081 1.236110 Cl -4.215697 -1.813183 2.441399
$\mathbf{I}_{CD}$ (X = Br) dual	
SCF Done: -3233.06455404 A.U. Br 4.754072 -1.098277 0.919514 C 2.066862 -0.182606 0.579980 C 1.720029 -1.672178 0.499586 C 1.532050 -2.376385 1.827590 O 0.535742 0.412809 0.435796 Y -0.909572 2.303575 -0.272662 Cl -3.359441 1.952304 -1.207522 Cl -0.412733 4.540144 0.683213 Cl 0.427833 2.148051 -2.376517 H 2.376296 0.220829 1.552457 H 2.404917 -2.204879 -0.180391 H 0.809279 -1.831670 2.469169 H 1.157979 -3.406072 1.669311 H 2.519814 -2.416257 2.327522 H 2.576220 0.265766 -0.286279 C -0.196026 -0.545915 -0.110928 O 0.375193 -1.703621 -0.217838 O -1.353902 -0.261173 -0.516323 Y -3.478555 -0.217966 0.514142 Cl -2.217157 1.448036 2.086082 Cl -2.769774 -2.387588 1.531249 Cl -5.957738 -0.398178 0.338492	
$\mathbf{I}_{AB}$ (X = I)	**B** (X = I)
SCF Done: -1623.59576757 A.U. I -2.627633 4.006047 1.244047 C -0.256286 1.770220 0.814757 C 0.724499 2.849273 0.788645 C -0.782674 1.092355 -0.410944 O 1.373506 1.551726 0.979808 Y 2.696275 0.174439 -0.130837 Cl 4.905378 0.116245 1.038431 Cl 1.484686 -2.014934 -0.179257 Cl 2.809093 1.275012 -2.371467 H 0.956681 3.329126 -0.180090 H 0.800366 3.512933 1.666349 H -0.210592 1.387086 -1.314624 H -1.838464 1.400692 -0.546704 H -0.746272 -0.011246 -0.295435 H -0.710574 1.536679 1.789034	SCF Done: -1623.62733104 A.U. Y 1.657129 0.062771 -0.328615 Cl 0.708473 0.621380 1.969366 Cl 4.138062 0.613804 -0.364524 O 0.700413 1.479691 -1.488644 C -1.238485 2.631805 -0.615026 C 0.047870 2.699680 -1.442937 H -1.764221 3.603088 -0.539777 H -0.211391 3.041422 -2.479348 C 0.946838 3.781657 -0.795309 H 1.907182 3.823157 -1.348086 H 0.479959 4.789954 -0.813255 H 1.170050 3.506240 0.257587 H -1.033056 2.204858 0.388258 Cl 1.175514 -2.299541 -1.129095 I -2.761832 1.247785 -1.494208
$\mathbf{I}_{BC}$ (X = I)	**C** (X = I)
SCF Done: -1812.09475957 A.U. Y 1.737496 -0.053947 0.122099 Cl 0.741872 -1.961672 1.467533 Cl 4.232079 0.343203 0.361450 O 0.709813 1.827423 0.015900 C -1.317192 3.042230 -0.534127 C 0.074628 2.581007 -0.971283 H -1.854519 3.587293 -1.333448 H -0.024131 1.962412 -1.898183 C 0.912496 3.829863 -1.319932 H 1.914864 3.496172 -1.656549 H 0.450022 4.430825 -2.131610 H 1.042299 4.470828 -0.423446	SCF Done: -1812.10184369 A.U. Y -4.004598 3.558681 -1.309709 Cl -5.426047 5.651559 -1.194740 Cl -3.146366 3.520282 -3.686719 Cl -5.563006 1.677836 -0.671447 O -2.573938 4.324811 0.398897 C -0.519823 0.819498 1.270849 C 0.186236 2.158160 1.027716 H -1.060465 0.450917 0.382581 H 0.875186 2.356331 1.875180 C 0.952676 2.256796 -0.290379 H 1.776058 1.515238 -0.312646 H 0.277328 2.072998 -1.148077

H -1.276459 3.642634 0.394020 O 1.516060 1.392515 2.384482 C 0.942603 2.399323 2.101524 O 0.434432 3.462950 2.186724 Cl 1.381000 -0.594971 -2.327582 I -2.647113 1.325665 -0.017486	H 1.392669 3.269042 -0.390314 H -1.197271 0.876660 2.142611 I 0.936530 -0.801451 1.806867 C -1.834051 3.295854 0.308627 O -2.053977 2.357853 -0.520946 O -0.777388 3.238958 1.169242
$\mathbf{I}_{CD}$ (X = I)	**D** (X = I)
SCF Done: -1812.08128581 A.U. Y -4.392107 4.005393 -1.366328 Cl -5.440722 6.099007 -0.480572 Cl -3.238367 4.412007 -3.547863 Cl -6.065738 2.150905 -1.476788 O -2.824136 3.447905 0.069069 C -0.142949 0.773098 0.397324 C 0.242947 2.084105 1.069523 H 0.315036 0.458868 -0.544664 H 0.535905 1.910275 2.120848 C 1.314812 2.861011 0.315543 H 2.257809 2.279841 0.312198 H 0.999882 3.036810 -0.733963 H 1.494918 3.839003 0.802906 H -0.822436 0.074274 0.897767 I 1.897677 -0.792724 1.552271 C -1.831046 2.660582 0.182537 O -1.600613 1.651745 -0.552229 O -0.962193 2.921665 1.176652	SCF Done: -1812.09426041 A.U. Y -4.498683 4.022540 -1.390589 Cl -5.490865 6.113866 -0.468761 Cl -3.325935 4.376539 -3.558940 Cl -6.142605 2.155165 -1.447762 O -2.857249 3.423761 0.002927 C -0.408454 0.956433 0.164591 C 0.212484 2.092403 1.001400 H 0.234581 0.601656 -0.658575 H 0.439134 1.759399 2.030512 C 1.385094 2.809016 0.364858 H 2.239115 2.101020 0.351961 H 1.151453 3.121443 -0.674806 H 1.669481 3.700764 0.957317 H -0.741833 0.092719 0.769369 I 2.143719 -0.847855 1.789393 C -1.845256 2.725983 0.213834 O -1.602468 1.601565 -0.435721 O -0.935399 3.050706 1.108312
$\mathbf{I}_{BC}$ (X = I) dual	**C** (X = I) dual
SCF Done: -3231.10011774 A.U. Y 2.908252 -1.656469 0.017657 Cl 1.994262 -0.863858 -2.223149 Cl 5.022423 -0.597122 0.894717 O 1.226386 -1.263643 1.221829 C 0.248038 0.869730 1.832593 C 0.696654 -0.533206 2.273275 H -0.256187 1.450041 2.626697 H 1.457858 -0.384858 3.082485 C -0.481578 -1.290831 2.921919 H -0.115479 -2.269863 3.290213 H -0.955256 -0.735079 3.754795 H -1.272031 -1.557584 2.179230 H -0.381677 0.825951 0.915027 I 1.939994 2.109645 1.132874 Cl 3.221629 -4.158645 0.063462 O -0.073449 -3.075489 -0.782503 C -0.557183 -2.036354 -0.588352 O -1.193008 -1.037528 -0.455258 Y -2.863878 0.054083 0.892337 Cl -3.720996 1.502643 -0.916970 Cl -3.062090 1.308955 3.041020 Cl -4.134771 -2.064226 1.108947	SCF Done: -3231.14918731 A.U. Y 2.646645 -1.741797 -0.454254 Cl 3.714459 -0.427575 -2.297224 Cl 3.898131 -1.282349 1.703174 O 0.702606 -1.270713 1.020165 C 0.168336 0.932726 2.031920 C 0.542147 -0.522728 2.272947 H 0.339318 1.519399 2.953639 H 1.578335 -0.581493 2.665861 C -0.419232 -1.233751 3.220621 H -0.079902 -2.277416 3.374381 H -0.413397 -0.722653 4.204618 H -1.462917 -1.256514 2.851306 H -0.871161 1.095129 1.688255 I 1.450051 1.865693 0.479931 Cl 2.883229 -4.202223 -0.801340 O 0.336729 -1.639716 -1.100273 C -0.203955 -1.274157 -0.035515 O -1.400600 -0.934016 0.182246 Y -3.499163 -0.421148 0.466773 Cl -4.910162 -0.731671 -1.567419 Cl -3.318049 1.945689 1.270036 Cl -4.191877 -1.867032 2.382835
$\mathbf{I}_{CD}$ (X = I) dual	
SCF Done: -3231.12776602 A.U. I 5.010757 -1.124779 0.874745 C 2.105579 -0.207192 0.555639 C 1.700777 -1.681472 0.502645 C 1.461415 -2.341643 1.846626 O 0.532488 0.424885 0.430061 Y -0.921234 2.312890 -0.256463 Cl -3.376533 1.957682 -1.178935 Cl -0.430411 4.538858 0.728172 Cl 0.412289 2.192885 -2.365900 H 2.414849 0.220097 1.517293 H 2.372651 -2.261356 -0.151899 H 0.749587 -1.750268 2.458217 H 1.045600 -3.357704 1.707126 H 2.430896 -2.413851 2.377047 H 2.580734 0.234179 -0.333081 C -0.191999 -0.527318 -0.124026 O 0.377712 -1.689213 -0.237777 O -1.350322 -0.249469 -0.537024 Y -3.462573 -0.240681 0.510633	

Cl -2.217018 1.423407 2.097722 Cl -2.707411 -2.398304 1.524093 Cl -5.936445 -0.472884 0.320727	
Model A:	
Y	**Y-PO**
SCF Done: -4301.87793092 A.U. Si -4.921890 2.344613 -0.331416 Si -3.405847 -1.452878 0.714733 Si -1.913412 -1.344322 -1.905821 Si -3.559763 2.339742 2.398372 Si -0.633820 -1.799915 2.189645 Si -2.989667 1.387007 -2.646869 Si -0.584218 1.371164 2.185835 O -2.145055 1.520657 2.721681 O -2.266771 -1.877327 1.848642 O -4.305072 1.547911 -1.659067 O -0.113041 -0.207951 2.253434 O -2.955636 -2.015031 -0.806320 O -2.689212 -0.238077 -2.889525 O -3.611828 2.742189 0.717808 O -0.758001 -0.483692 -1.024000 O -1.638551 1.950885 -1.780926 O -0.628476 1.805594 0.542439 H -5.773378 1.363033 0.407638 H -3.495107 0.036763 0.647899 H -4.699694 -2.091374 1.077009 H -0.439850 -2.407512 3.538250 H -5.664557 3.573368 -0.703246 H -4.679208 1.374073 2.623712 H 0.153321 -2.495974 1.128466 H -3.705491 3.570283 3.213341 Si -0.396279 1.127163 -0.975535 O 1.114825 1.345596 -1.550639 H 0.389523 2.206727 2.910366 H -3.137655 2.073046 -3.942089 H -1.287220 -2.399829 -2.727627 Y -1.617267 3.944247 -0.296560 O 0.224510 4.052363 -1.168290 C 1.998865 2.446847 -1.264306 C 1.452738 3.789760 -1.773026 H 2.161505 2.513187 -0.164384 H 2.964253 2.201735 -1.751806 H 1.309983 3.693030 -2.880386 C 2.454435 4.916423 -1.494545 H 3.426222 4.740145 -2.001312 H 2.039227 5.876847 -1.858235 H 2.629389 5.013489 -0.402550 Cl -1.296107 4.791484 2.079096 Cl -3.333819 4.871919 -1.925106	SCF Done: -4494.89180489 A.U. Si -4.911610 2.282310 -0.339048 Si -3.408723 -1.468304 0.710986 Si -1.903375 -1.346410 -1.899280 Si -3.557069 2.334945 2.383209 Si -0.636341 -1.822722 2.158989 Si -2.982842 1.375916 -2.641202 Si -0.601412 1.360177 2.181238 O -2.172706 1.463116 2.704446 O -2.269621 -1.941205 1.827449 O -4.292991 1.422683 -1.626699 O -0.136042 -0.227307 2.199924 O -2.978891 -2.007038 -0.824419 O -2.631947 -0.242035 -2.914095 O -3.617209 2.752833 0.704413 O -0.768745 -0.489596 -0.985012 O -1.632726 1.949654 -1.777140 O -0.615768 1.830081 0.548077 H -5.746266 1.316052 0.438828 H -3.473788 0.022021 0.684508 H -4.710108 -2.096405 1.067063 H -0.428370 -2.415951 3.513376 H -5.692957 3.476964 -0.743547 H -4.698318 1.394464 2.608593 H 0.158108 -2.526308 1.107360 H -3.689898 3.560221 3.208555 Si -0.411278 1.123406 -0.955016 O 1.101525 1.331334 -1.541100 H 0.378730 2.138234 2.956918 H -3.167677 2.033249 -3.944719 H -1.257555 -2.413358 -2.692341 Y -1.629479 4.007829 -0.320685 O 0.232210 4.085948 -1.206142 C 1.979200 2.431938 -1.257819 C 1.449317 3.766883 -1.804271 H 2.122925 2.523525 -0.156627 H 2.954495 2.178520 -1.721985 H 1.302905 3.632979 -2.908250 C 2.485450 4.876139 -1.574983 H 3.452933 4.650497 -2.070622 H 2.106969 5.834724 -1.982701 H 2.666293 5.011807 -0.487554 Cl -1.199735 4.561148 2.170536 Cl -3.407686 4.522630 -2.156845 O -1.565374 6.383227 -0.404583 C -0.397102 7.223541 -0.246148 C -1.045458 7.094736 -1.571620 H 0.536373 6.671238 -0.044567 H -0.582114 8.120363 0.370277 H -0.556600 6.401127 -2.281522 C -1.968174 8.124760 -2.158840 H -1.414280 8.769429 -2.872621 H -2.785111 7.615067 -2.708253 H -2.413132 8.762961 -1.370048
$\mathbf{I}_{\mathbf{AB}}$ (X = Br)	**B** (X = Br)
CF Done: -4508.46401208 A.U. Si -4.915697 2.470112 0.370894 Si -3.179669 -1.259218 0.287401 Si -2.189742 -0.508625 -2.473364 Si -3.225503 2.407657 2.882943 Si -0.274528 -1.763728 1.278962 Si -3.349267 2.176780 -2.334470 Si -0.462871 1.304392 2.074719 O -1.863719 1.448505 2.966442 O -1.905009 -2.048316 1.027775 O -4.482775 1.918737 -1.138823	SCF Done: -4508.46401208 A.U. Si -4.915697 2.470112 0.370894 Si -3.179669 -1.259218 0.287401 Si -2.189742 -0.508625 -2.473364 Si -3.225503 2.407657 2.882943 Si -0.274528 -1.763728 1.278962 Si -3.349267 2.176780 -2.334470 Si -0.462871 1.304392 2.074719 O -1.863719 1.448505 2.966442 O -1.905009 -2.048316 1.027775 O -4.482775 1.918737 -1.138823

O -0.030165 -0.302726 2.037793	O -0.030165 -0.302726 2.037793
O -3.064587 -1.417511 -1.377004	O -3.064587 -1.417511 -1.377004
O -3.146188 0.701723 -3.113960	O -3.146188 0.701723 -3.113960
O -3.550987 2.927518 1.291172	O -3.550987 2.927518 1.291172
O -0.911151 0.180198 -1.685943	O -0.911151 0.180198 -1.685943
O -1.879289 2.561587 -1.630386	O -1.879289 2.561587 -1.630386
O -0.853542 1.836151 0.549817	O -0.853542 1.836151 0.549817
H -5.507188 1.279271 1.069474	H -5.507188 1.279271 1.069474
H -3.153800 0.176448 0.686390	H -3.153800 0.176448 0.686390
H -4.434847 -1.949360 0.709336	H -4.434847 -1.949360 0.709336
H 0.198265 -2.830027 2.219628	H 0.198265 -2.830027 2.219628
H -5.922400 3.565223 0.320434	H -5.922400 3.565223 0.320434
H -4.373467 1.524440 3.282007	H -4.373467 1.524440 3.282007
H 0.467915 -1.811287 -0.016180	H 0.467915 -1.811287 -0.016180
H -3.143142 3.584770 3.787974	H -3.143142 3.584770 3.787974
Si -0.379095 1.679416 -1.086565	Si -0.379095 1.679416 -1.086565
O 1.241124 1.092739 -1.031972	O 1.241124 1.092739 -1.031972
H 0.678514 2.011062 2.695253	H 0.678514 2.011062 2.695253
H -3.783040 3.151781 -3.355970	H -3.783040 3.151781 -3.355970
H -1.750149 -1.407682 -3.570000	H -1.750149 -1.407682 -3.570000
Y -1.552877 4.361954 -0.101889	Y -1.552877 4.361954 -0.101889
O 0.281953 3.344070 -1.240286	O 0.281953 3.344070 -1.240286
C 2.154787 2.063993 -0.576081	C 2.154787 2.063993 -0.576081
C 1.706802 3.440586 -1.121454	C 1.706802 3.440586 -1.121454
H 2.172275 2.102606 0.543500	H 2.172275 2.102606 0.543500
H 3.183088 1.812035 -0.917885	H 3.183088 1.812035 -0.917885
H 2.109671 3.579608 -2.153795	H 2.109671 3.579608 -2.153795
C 2.123755 4.610191 -0.242181	C 2.123755 4.610191 -0.242181
H 3.232009 4.662405 -0.181692	H 3.232009 4.662405 -0.181692
H 1.732709 5.565491 -0.641792	H 1.732709 5.565491 -0.641792
H 1.718056 4.493124 0.785106	H 1.718056 4.493124 0.785106
Cl -0.821450 4.634879 2.363146	Cl -0.821450 4.634879 2.363146
Cl -3.876554 5.120050 -1.027811	Cl -3.876554 5.120050 -1.027811
O -0.719273 6.133631 -0.811822	O -0.719273 6.133631 -0.811822
C -1.709384 7.979994 -1.775229	C -1.709384 7.979994 -1.775229
C -0.618329 6.921206 -1.957638	C -0.618329 6.921206 -1.957638
H -1.572053 8.528733 -0.826477	H -1.572053 8.528733 -0.826477
H -2.719994 7.532396 -1.831648	H -2.719994 7.532396 -1.831648
H 0.376330 7.440477 -1.986862	H 0.376330 7.440477 -1.986862
C -0.779573 6.090237 -3.238424	C -0.779573 6.090237 -3.238424
H -0.661723 6.707707 -4.152489	H -0.661723 6.707707 -4.152489
H -0.022882 5.280041 -3.246109	H -0.022882 5.280041 -3.246109
H -1.786269 5.620241 -3.253096	H -1.786269 5.620241 -3.253096
Br -1.680814 9.449805 -3.220473	Br -1.680814 9.449805 -3.220473
$\mathbf{I}_{BC}$ (X = Br)	**C** (X = Br)
SCF Done: -4696.91712518 A.U.	SCF Done: -4696.92251602 A.U.
Si -4.474402 1.809786 0.753833	Si -5.189055 1.920963 -0.402370
Si -2.426163 -1.174017 2.660997	Si -3.110314 -1.493940 0.849866
Si -1.237991 -1.807259 -0.034541	Si -1.619306 -1.259620 -1.773780
Si -2.850462 3.004654 3.024089	Si -3.792793 2.396519 2.271108
Si 0.446741 -0.836577 3.814089	Si -0.369878 -1.346586 2.305850
Si -2.772203 0.385228 -1.412517	Si -3.206297 1.175228 -2.656096
Si 0.122525 2.176730 2.784809	Si -0.745932 1.819684 2.116937
O -1.375832 2.370664 3.484740	O -2.317229 1.719997 2.660154
O -1.178274 -1.233055 3.768819	O -1.980062 -1.731396 2.054159
O -3.926995 0.570761 -0.222550	O -4.520344 1.021619 -1.640397
O 0.736596 0.730069 3.352731	O -0.093696 0.287512 2.274479
O -2.079455 -2.174483 1.357624	O -2.508512 -2.058631 -0.612817
O -2.236804 -1.214260 -1.219639	O -2.592908 -0.400559 -2.804520
O -3.153145 2.734308 1.352451	O -3.932524 2.593153 0.564647
O -0.122772 -0.615136 0.351860	O -0.601068 -0.177925 -0.989406
O -1.413785 1.308948 -1.010903	O -1.977043 1.984788 -1.819739
O -0.112770 2.004438 1.138913	O -0.800552 2.144809 0.473756
H -5.057244 1.113363 1.948509	H -5.891466 0.925006 0.471662
H -2.592475 0.226974 2.188505	H -3.418862 -0.042007 0.727894
H -3.647498 -1.708828 3.330438	H -4.312693 -2.307553 1.194609
H 0.871093 -0.998376 5.241935	H -0.032678 -1.865963 3.669987
H -5.497128 2.687187 0.130091	H -6.116197 2.986225 -0.856016
H -3.868024 2.176819 3.753830	H -4.809632 1.354211 2.633430
H 1.222981 -1.757275 2.923835	H 0.478642 -2.002815 1.261190
H -3.018557 4.441307 3.354839	H -4.067841 3.679001 2.962424

Si	-0.013392	0.975569	-0.153280	Si	-0.584164	1.489688	-1.028895
O	1.425216	1.093545	-0.947299	O	0.844811	1.929286	-1.711949
H	1.138839	3.183813	3.136442	H	0.160172	2.694276	2.879963
H	-3.220534	0.438356	-2.813915	H	-3.471753	1.571820	-4.048341
H	-0.563900	-3.040117	-0.509461	H	-0.837243	-2.267888	-2.529061
O	0.207751	3.575339	-1.309198	O	-0.548936	4.426489	-1.474870
C	2.197001	2.299905	-0.975159	C	1.496772	3.189622	-1.499674
C	1.500787	3.414496	-1.777740	C	0.693954	4.367676	-2.078568
H	2.366929	2.661588	0.066182	H	1.641526	3.359623	-0.407382
H	3.180449	2.043378	-1.423582	H	2.493378	3.112555	-1.984579
H	1.476897	3.082760	-2.850986	H	0.578839	4.166673	-3.178969
C	2.312325	4.713471	-1.676221	C	1.480677	5.676104	-1.902139
H	3.361158	4.579096	-2.019707	H	2.496852	5.618780	-2.349129
H	1.849524	5.509332	-2.292164	H	0.940627	6.510783	-2.392154
H	2.321792	5.066956	-0.623614	H	1.573994	5.923195	-0.823830
Y	-1.616202	3.946679	-0.392486	Y	-2.417453	4.279452	-0.563281
Cl	-3.618275	3.144308	-1.965414	Cl	-4.052729	3.981679	-2.642859
Cl	-0.673551	5.030246	1.835979	Cl	-1.589079	4.756500	1.927688
O	-1.826633	5.930831	-1.245438	O	-2.593233	6.607285	-0.731902
C	-0.981238	6.763137	-1.998065	C	-1.657425	7.690564	-0.894970
H	-0.260357	6.129944	-2.571798	H	-0.794180	7.203237	-1.391776
C	-1.777971	7.619386	-2.986395	C	-2.227384	8.791803	-1.783496
H	-1.106059	8.240242	-3.613678	H	-1.460942	9.572496	-1.964218
H	-2.369135	6.951934	-3.645295	H	-2.531452	8.360141	-2.758045
H	-2.479323	8.284373	-2.443450	H	-3.114179	9.247668	-1.302691
C	-0.190122	7.560076	-0.957975	C	-1.222227	8.126748	0.504004
H	0.340007	6.889399	-0.258513	H	-0.948024	7.249888	1.121415
H	-0.830263	8.271190	-0.404073	H	-1.981413	8.747839	1.011063
Br	1.291719	8.721819	-1.785996	Br	0.460662	9.273074	0.414949
C	-3.380364	6.621113	0.022172	C	-3.877160	6.747056	0.066882
O	-3.425853	7.794778	-0.128785	O	-4.243044	7.865729	0.380321
O	-3.658532	5.539090	0.448750	O	-4.289008	5.568517	0.235624
I_{CD} (X = Br)				**D** (X = Br)			
SCF Done: -4696.92251602 A.U.				SCF Done: -4696.92251602 A.U.			
Si	-5.189055	1.920963	-0.402370	Si	-5.189055	1.920963	-0.402370
Si	-3.110314	-1.493940	0.849866	Si	-3.110314	-1.493940	0.849866
Si	-1.619306	-1.259620	-1.773780	Si	-1.619306	-1.259620	-1.773780
Si	-3.792793	2.396519	2.271108	Si	-3.792793	2.396519	2.271108
Si	-0.369878	-1.346586	2.305850	Si	-0.369878	-1.346586	2.305850
Si	-3.206297	1.175228	-2.656096	Si	-3.206297	1.175228	-2.656096
Si	-0.745932	1.819684	2.116937	Si	-0.745932	1.819684	2.116937
O	-2.317229	1.719997	2.660154	O	-2.317229	1.719997	2.660154
O	-1.980062	-1.731396	2.054159	O	-1.980062	-1.731396	2.054159
O	-4.520344	1.021619	-1.640397	O	-4.520344	1.021619	-1.640397
O	-0.093696	0.287512	2.274479	O	-0.093696	0.287512	2.274479
O	-2.508512	-2.058631	-0.612817	O	-2.508512	-2.058631	-0.612817
O	-2.592908	-0.400559	-2.804520	O	-2.592908	-0.400559	-2.804520
O	-3.932524	2.593153	0.564647	O	-3.932524	2.593153	0.564647
O	-0.601068	-0.177925	-0.989406	O	-0.601068	-0.177925	-0.989406
O	-1.977043	1.984788	-1.819739	O	-1.977043	1.984788	-1.819739
O	-0.800552	2.144809	0.473756	O	-0.800552	2.144809	0.473756
H	-5.891466	0.925006	0.471662	H	-5.891466	0.925006	0.471662
H	-3.418862	-0.042007	0.727894	H	-3.418862	-0.042007	0.727894
H	-4.312693	-2.307553	1.194609	H	-4.312693	-2.307553	1.194609
H	-0.032678	-1.865963	3.669987	H	-0.032678	-1.865963	3.669987
H	-6.116197	2.986225	-0.856016	H	-6.116197	2.986225	-0.856016
H	-4.809632	1.354211	2.633430	H	-4.809632	1.354211	2.633430
H	0.478642	-2.002815	1.261190	H	0.478642	-2.002815	1.261190
H	-4.067841	3.679001	2.962424	H	-4.067841	3.679001	2.962424
Si	-0.584164	1.489688	-1.028895	Si	-0.584164	1.489688	-1.028895
O	0.844811	1.929286	-1.711949	O	0.844811	1.929286	-1.711949
H	0.160172	2.694276	2.879963	H	0.160172	2.694276	2.879963
H	-3.471753	1.571820	-4.048341	H	-3.471753	1.571820	-4.048341
H	-0.837243	-2.267888	-2.529061	H	-0.837243	-2.267888	-2.529061
O	-0.548936	4.426489	-1.474870	O	-0.548936	4.426489	-1.474870
C	1.496772	3.189622	-1.499674	C	1.496772	3.189622	-1.499674
C	0.693954	4.367676	-2.078568	C	0.693954	4.367676	-2.078568
H	1.641526	3.359623	-0.407382	H	1.641526	3.359623	-0.407382
H	2.493378	3.112555	-1.984579	H	2.493378	3.112555	-1.984579
H	0.578839	4.166673	-3.178969	H	0.578839	4.166673	-3.178969
C	1.480677	5.676104	-1.902139	C	1.480677	5.676104	-1.902139

H 2.496852 5.618780 -2.349129	H 2.496852 5.618780 -2.349129
H 0.940627 6.510783 -2.392154	H 0.940627 6.510783 -2.392154
H 1.573994 5.923195 -0.823830	H 1.573994 5.923195 -0.823830
Y -2.417453 4.279452 -0.563281	Y -2.417453 4.279452 -0.563281
Cl -4.052729 3.981679 -2.642859	Cl -4.052729 3.981679 -2.642859
Cl -1.589079 4.756500 1.927688	Cl -1.589079 4.756500 1.927688
O -2.593233 6.607285 -0.731902	O -2.593233 6.607285 -0.731902
C -1.657425 7.690564 -0.894970	C -1.657425 7.690564 -0.894970
H -0.794180 7.203237 -1.391776	H -0.794180 7.203237 -1.391776
C -2.227384 8.791803 -1.783496	C -2.227384 8.791803 -1.783496
H -1.460942 9.572496 -1.964218	H -1.460942 9.572496 -1.964218
H -2.531452 8.360141 -2.758045	H -2.531452 8.360141 -2.758045
H -3.114179 9.247668 -1.302691	H -3.114179 9.247668 -1.302691
C -1.222227 8.126748 0.504004	C -1.222227 8.126748 0.504004
H -0.948024 7.249888 1.121415	H -0.948024 7.249888 1.121415
H -1.981413 8.747839 1.011063	H -1.981413 8.747839 1.011063
Br 0.460662 9.273074 0.414949	Br 0.460662 9.273074 0.414949
C -3.877160 6.747056 0.066882	C -3.877160 6.747056 0.066882
O -4.243044 7.865729 0.380321	O -4.243044 7.865729 0.380321
O -4.289008 5.568517 0.235624	O -4.289008 5.568517 0.235624
I_{AB} (X = I)	**B** (X = I)
SCF Done: -4506.49791039 A.U.	SCF Done: -4506.52647377 A.U.
Si -6.403005 6.487517 1.137827	Si -4.916808 2.468337 0.367711
Si -7.796924 2.643084 1.057256	Si -3.178663 -1.261586 0.292126
Si -6.904610 2.577036 -1.835031	Si -2.189758 -0.515636 -2.470099
Si -4.977640 5.103091 3.423380	Si -3.226935 2.406023 2.879783
Si -6.007641 0.179138 1.703169	Si -0.271575 -1.762236 1.280554
Si -5.851590 5.309007 -1.726760	Si -3.350409 2.169634 -2.337487
Si -3.853947 2.434578 2.345212	Si -0.462545 1.306911 2.072939
O -4.631561 3.473920 3.389944	O -1.863893 1.448737 2.964182
O -7.358597 1.165377 1.702211	O -1.902432 -2.047641 1.032914
O -6.663428 5.882653 -0.388242	O -4.483297 1.914238 -1.140729
O -4.677220 0.997680 2.286770	O -0.026487 -0.299027 2.035104
O -8.022570 2.504441 -0.596795	O -3.064484 -1.422551 -1.372109
O -6.817280 4.138220 -2.432282	O -3.146502 0.693046 -3.113492
O -5.004071 5.772748 1.841430	O -3.551459 2.926361 1.287426
O -5.424138 2.161310 -1.224343	O -0.912096 0.175785 -1.683270
O -4.458598 4.533471 -1.198600	O -1.880606 2.556914 -1.633990
O -3.910641 3.197954 0.861955	O -0.854544 1.838479 0.547854
H -7.560980 6.019159 1.966677	H -5.509422 1.279361 1.068208
H -6.721186 3.633169 1.353937	H -3.154456 0.174918 0.688406
H -9.107525 3.025848 1.658261	H -4.432715 -1.952391 0.716178
H -6.293071 -0.934718 2.660889	H 0.203126 -2.825882 2.223184
H -6.313669 7.970731 1.173156	H -5.921607 3.564981 0.315035
H -6.373946 5.232813 3.953247	H -4.374169 1.520855 3.276240
H -5.727643 -0.332498 0.328429	H 0.468794 -1.812660 -0.015615
H -4.016639 5.864225 4.263864	H -3.147842 3.582525 3.785831
Si -3.919898 2.836498 -0.822399	Si -0.380055 1.676786 -1.088611
O -3.157785 1.313064 -1.000117	O 1.240063 1.090832 -1.033164
H -2.481789 2.110784 2.791314	H 0.677666 2.015887 2.692870
H -5.581688 6.356993 -2.731045	H -3.785137 3.142087 -3.360968
H -7.341689 1.666738 -2.920580	H -1.749093 -1.416593 -3.564688
Y -2.896916 5.476750 0.276582	Y -1.557137 4.355120 -0.103009
O -2.311690 3.622369 -1.093258	O 0.280020 3.341946 -1.244054
C -1.778544 1.343185 -0.705741	C 2.153317 2.062766 -0.577856
C -1.206517 2.707553 -1.163590	C 1.704877 3.439083 -1.123642
H -1.607897 1.221315 0.394005	H 2.170941 2.101605 0.541688
H -1.263015 0.502485 -1.218859	H 3.181655 1.811125 -0.919687
H -0.910334 2.647149 -2.237558	H 2.108612 3.578403 -2.155557
C -0.022988 3.161443 -0.321817	C 2.121245 4.608255 -0.243513
H 0.787023 2.403352 -0.375993	H 3.229427 4.658270 -0.180036
H 0.377831 4.131928 -0.669698	H 1.733669 5.564485 -0.644131
H -0.319916 3.283825 0.741106	H 1.712689 4.492211 0.782754
Cl -1.751812 5.124274 2.536654	Cl -0.828673 4.634946 2.361474
Cl -3.917157 7.735443 -0.418326	Cl -3.875515 5.117571 -1.035826
O -1.042586 6.182665 -0.758543	O -0.715257 6.127692 -0.811426
C -0.475401 7.565856 -1.468575	C -1.692613 7.983638 -1.745974
C -0.701827 6.305682 -2.173316	C -0.611888 6.917416 -1.956045
H 0.500626 7.790285 -1.023047	H -1.543856 8.513137 -0.788109
H -1.274965 8.319237 -1.437480	H -2.708128 7.546575 -1.802863
H 0.207734 5.722225 -2.419872	H 0.390291 7.421296 -1.988887

C -1.825359 6.152150 -3.167258	C -0.792969 6.086955 -3.234669
H -1.479099 6.536409 -4.147910	H -0.667527 6.693837 -4.154807
H -2.119939 5.088086 -3.260624	H -0.049178 5.264721 -3.240724
H -2.706206 6.745720 -2.850761	H -1.806027 5.630742 -3.242644
I 0.782319 9.162592 -3.795384	I -1.683156 9.649388 -3.286899
I_{BC} (X = I)	**C** (X = I)
SCF Done: -4694.97904710 A.U.	SCF Done: -4694.98387303 A.U.
Si -4.470969 1.814077 0.754273	Si -5.166667 1.916645 -0.289702
Si -2.431387 -1.176561 2.659331	Si -3.102314 -1.446783 0.790361
Si -1.243663 -1.810719 -0.036267	Si -1.735248 -1.244679 -1.897339
Si -2.844655 3.004406 3.025990	Si -3.692772 2.434516 2.336511
Si 0.441648 -0.846467 3.813848	Si -0.323830 -1.387788 2.164438
Si -2.772428 0.386319 -1.413102	Si -3.309824 1.215067 -2.682392
Si 0.125576 2.168801 2.786547	Si -0.691039 1.789955 2.012111
O -1.371619 2.367580 3.487688	O -2.212250 1.743784 2.688420
O -1.184321 -1.239036 3.767809	O -1.935850 -1.777673 1.938656
O -3.927708 0.574967 -0.224198	O -4.530352 1.036024 -1.556881
O 0.735164 0.719277 3.351642	O -0.055650 0.248216 2.127491
O -2.086220 -2.176895 1.355421	O -2.603512 -2.022919 -0.705945
O -2.241044 -1.214388 -1.221007	O -2.720831 -0.364275 -2.897973
O -3.146006 2.732647 1.354190	O -3.888783 2.607857 0.633775
O -0.125769 -0.621333 0.351249	O -0.669904 -0.186146 -1.143869
O -1.412528 1.306856 -1.009979	O -2.003005 2.009657 -1.955877
O -0.113486 1.998707 1.140679	O -0.906798 2.097198 0.376546
H -5.056282 1.118459 1.948134	H -5.810806 0.899175 0.604779
H -2.594029 0.225131 2.187442	H -3.310088 0.025560 0.712676
H -3.654421 -1.708860 3.327600	H -4.337922 -2.187174 1.178067
H 0.864781 -1.008636 5.241967	H 0.040112 -1.906909 3.521759
H -5.489616 2.696294 0.130783	H -6.138978 2.961379 -0.694685
H -3.865172 2.180571 3.755930	H -4.713661 1.416731 2.752860
H 1.216109 -1.769162 2.924156	H 0.511646 -2.035792 1.104254
H -3.007522 4.442462 3.353057	H -3.914751 3.735591 3.011971
Si -0.013664 0.969714 -0.151601	Si -0.638772 1.482347 -1.141378
O 1.426110 1.087928 -0.943319	O 0.827949 1.928137 -1.738294
H 1.145785 3.171852 3.138136	H 0.301771 2.650227 2.677578
H -3.220304 0.442613 -2.814489	H -3.687817 1.624879 -4.044544
H -0.572165 -3.044542 -0.512192	H -0.997530 -2.268585 -2.676014
O 0.209998 3.571606 -1.307078	O -0.526067 4.387113 -1.474602
C 2.197958 2.294455 -0.967336	C 1.503641 3.123187 -1.322240
C 1.504524 3.409492 -1.771351	C 0.810547 4.401145 -1.833008
H 2.364432 2.655164 0.074855	H 1.547787 3.161894 -0.208714
H 3.182900 2.038497 -1.412724	H 2.541350 3.054843 -1.712692
H 1.483694 3.078280 -2.844749	H 0.905106 4.400394 -2.953009
C 2.314602 4.708687 -1.666063	C 1.541969 5.630846 -1.273538
H 3.364300 4.577754 -2.007959	H 2.626762 5.622869 -1.516716
H 1.850390 5.502744 -2.283165	H 1.109423 6.561496 -1.690326
H 2.320452 5.060550 -0.612882	H 1.419649 5.666965 -0.170703
Y -1.609975 3.945103 -0.384642	Y -2.391263 4.271180 -0.550464
Cl -3.608922 3.151649 -1.965243	Cl -4.156109 3.993255 -2.533855
Cl -0.654348 5.027091 1.837635	Cl -1.431344 4.770995 1.879675
O -1.819990 5.937323 -1.238120	O -2.611011 6.585899 -0.795809
C -0.988792 6.774549 -2.003459	C -1.745073 7.684751 -1.142628
H -0.265438 6.141267 -2.573454	H -0.947258 7.199672 -1.743195
C -1.809430 7.605479 -2.993976	C -2.477915 8.723132 -1.987793
H -1.161793 8.232513 -3.640246	H -1.776943 9.508358 -2.335714
H -2.394661 6.916782 -3.636068	H -2.917749 8.223301 -2.873975
H -2.519094 8.262149 -2.452076	H -3.293257 9.187259 -1.401463
C -0.207607 7.580425 -0.960787	C -1.147269 8.173304 0.176827
H 0.330891 6.911125 -0.265590	H -0.715748 7.326044 0.742636
H -0.856674 8.278117 -0.399948	H -1.884967 8.720482 0.791013
I 1.413460 8.896840 -1.827141	I 0.551709 9.601797 -0.115236
C -3.365008 6.609970 0.010414	C -3.835306 6.746185 0.108721
O -3.434742 7.782997 -0.141781	O -4.192073 7.872784 0.399638
O -3.633625 5.529115 0.450142	O -4.204547 5.571510 0.363925
I_{CD} (X = I)	**D** (X = I)
SCF Done: -4694.96716511 A.U.	SCF Done: -4694.98250351 A.U.
Si -4.286875 1.868976 -1.563223	Si -4.311662 1.835032 -1.552210
Si -1.872905 -1.510529 -1.072117	Si -1.848368 -1.492598 -1.099799
Si -0.336090 -0.480290 -3.454686	Si -0.349438 -0.441123 -3.499329
Si -3.070633 1.745937 1.232516	Si -3.098991 1.726804 1.240932
Si 0.789650 -1.456113 0.546149	Si 0.833125 -1.399347 0.502564

Si -2.142276 1.927359 -3.801667	Si -2.168245 1.951763 -3.811665
Si 0.025236 1.585287 1.131141	Si 0.000640 1.619775 1.105074
O -1.534722 1.165711 1.535018	O -1.546358 1.181597 1.527163
O -0.746967 -1.930768 0.083998	O -0.690753 -1.899458 0.028230
O -3.457696 1.388366 -2.930283	O -3.457379 1.396763 -2.918360
O 0.867646 0.159953 0.919005	O 0.873616 0.221044 0.877870
O -1.190727 -1.628206 -2.602894	O -1.201112 -1.588612 -2.648316
O -1.344248 0.522650 -4.311402	O -1.358753 0.570753 -4.349182
O -3.168877 2.399772 -0.362063	O -3.216530 2.401080 -0.345157
O 0.505360 0.455574 -2.339553	O 0.487450 0.495148 -2.377091
O -1.039095 2.623767 -2.721153	O -1.054502 2.671637 -2.752696
O -0.035458 2.324015 -0.380511	O -0.100472 2.358352 -0.411877
H -4.904410 0.616561 -1.018938	H -4.878784 0.555168 -1.019097
H -2.322576 -0.109015 -0.845385	H -2.310312 -0.098114 -0.853644
H -2.992276 -2.493033 -0.993938	H -2.951539 -2.490481 -1.005380
H 1.115086 -2.249286 1.773752	H 1.166380 -2.183774 1.732182
H -5.313025 2.912329 -1.805871	H -5.381487 2.833310 -1.794042
H -3.951613 0.532564 1.217247	H -3.949747 0.493260 1.212072
H 1.765051 -1.742018 -0.552438	H 1.820066 -1.655424 -0.591848
H -3.550066 2.739378 2.224180	H -3.595593 2.694178 2.249139
Si 0.360901 2.075218 -1.975720	Si 0.341741 2.107210 -2.001600
O 1.781551 2.777343 -2.407867	O 1.759778 2.827464 -2.395334
H 0.786478 2.344014 2.136969	H 0.745177 2.421362 2.089714
H -2.421891 2.657446 -5.048625	H -2.489215 2.726741 -5.020568
H 0.594583 -1.174651 -4.375514	H 0.583874 -1.122053 -4.425404
O 0.124595 4.952552 -1.672672	O 0.097708 5.004909 -1.655795
C 2.299366 3.995621 -1.852868	C 2.272382 4.034163 -1.803785
C 1.396757 5.202462 -2.159956	C 1.390038 5.255157 -2.106770
H 2.394567 3.891888 -0.747006	H 2.343388 3.906013 -0.699050
H 3.312590 4.133761 -2.285849	H 3.295147 4.172818 -2.211306
H 1.362455 5.308630 -3.278018	H 1.377560 5.386905 -3.220675
C 1.990859 6.483901 -1.559306	C 1.975195 6.515550 -1.458777
H 3.016500 6.685674 -1.936224	H 3.012429 6.713120 -1.803005
H 1.354137 7.353063 -1.817610	H 1.360514 7.401670 -1.712153
H 2.021430 6.403869 -0.452332	H 1.976774 6.408176 -0.353856
Y -1.717820 4.396993 -0.917662	Y -1.706140 4.363341 -0.934057
Cl -3.294960 4.546188 -3.061679	Cl -3.416594 4.573929 -2.930015
Cl -1.220718 4.347126 1.658408	Cl -1.356211 4.388255 1.644282
O -2.129101 6.772815 -0.707656	O -2.229189 6.711965 -0.674470
C -1.790027 8.074531 -1.291133	C -1.844506 8.024093 -1.260433
H -0.757970 8.260250 -0.941707	H -0.854628 8.279339 -0.841504
C -1.855558 7.974549 -2.807038	C -1.809554 7.907677 -2.769408
H -1.527875 8.933154 -3.254687	H -1.469053 8.881731 -3.175623
H -1.192704 7.157924 -3.153351	H -1.095532 7.115446 -3.069155
H -2.887946 7.743414 -3.137517	H -2.808804 7.652557 -3.176086
C -2.742524 9.092703 -0.673885	C -2.953630 8.919015 -0.667468
H -2.656009 9.350419 0.386783	H -2.627286 9.464762 0.237720
H -3.451727 9.652009 -1.290148	H -3.372928 9.637350 -1.392487
I -1.099500 11.348662 -1.068761	I -0.540781 11.435860 -1.362124
C -3.473138 6.650240 -0.311528	C -3.533637 6.736724 -0.244253
O -4.120488 7.736683 -0.293525	O -4.021283 7.970934 -0.288549
O -3.796758 5.476762 -0.049805	O -4.087136 5.711723 0.100402
(OH) **Y**	(OH) **Y-PO**
SCF Done: -4527.56884383 A.U.	SCF Done: -4720.58358104 A.U.
Si -4.915878 2.267370 -0.320580	Si -4.893934 2.238087 -0.325966
Si -3.328972 -1.460535 0.729262	Si -3.357340 -1.505477 0.714600
Si -1.964183 -1.366533 -1.951628	Si -1.906131 -1.366865 -1.908883
Si -3.523492 2.373441 2.391366	Si -3.516980 2.322093 2.383687
Si -0.460330 -1.747608 2.108307	Si -0.528816 -1.830954 2.101721
Si -3.025315 1.318115 -2.677764	Si -2.990276 1.306996 -2.656057
Si -0.563602 1.408068 2.115152	Si -0.566466 1.337972 2.137260
O -2.108026 1.555544 2.699502	O -2.126582 1.462196 2.689523
O -2.078540 -1.900011 1.729696	O -2.158176 -1.980958 1.762389
O -4.271257 1.414902 -1.591449	O -4.262392 1.371098 -1.594421
O -0.025802 -0.131927 2.230001	O -0.070824 -0.223019 2.157570
O -3.049563 -1.960373 -0.851435	O -3.013364 -2.003549 -0.854332
O -2.715611 -0.282098 -2.975479	O -2.645022 -0.290665 -2.943721
O -3.616217 2.756229 0.705648	O -3.602755 2.748638 0.705460
O -0.791251 -0.535022 -1.086782	O -0.785053 -0.511063 -1.003060
O -1.648160 1.898044 -1.863637	O -1.647159 1.920272 -1.809584
O -0.731947 1.769846 0.461871	O -0.669650 1.816028 0.510184

H -5.764158 1.326312 0.469722 H -3.441515 0.028610 0.735228 H -4.572889 -2.131954 1.194305 H -0.260837 -2.376379 3.445995 H -5.654856 3.474957 -0.767960 H -4.652885 1.434363 2.666210 H 0.382166 -2.367555 1.044762 H -3.623878 3.630444 3.174114 Si -0.427123 1.071828 -1.034883 O 1.107065 1.300396 -1.534916 O 0.524782 2.426390 2.796147 H 0.216874 3.365298 2.712313 O -3.268497 2.144720 -4.066864 H -3.364366 3.108604 -3.867050 O -1.202416 -2.553457 -2.793257 H -1.770101 -3.137280 -3.327270 Y -1.640415 3.888510 -0.415871 O 0.211944 4.012598 -1.232372 C 1.972677 2.387771 -1.151556 C 1.496981 3.737350 -1.709198 H 2.024827 2.446979 -0.040780 H 2.978682 2.133477 -1.541847 H 1.460888 3.646725 -2.824324 C 2.473556 4.853084 -1.322495 H 3.489608 4.668892 -1.729370 H 2.107778 5.820284 -1.719759 H 2.539610 4.940366 -0.217846 Cl -1.253293 4.900092 1.921308 Cl -3.339964 4.758559 -2.143880	H -5.730831 1.292907 0.472513 H -3.443446 -0.015098 0.725051 H -4.631661 -2.157419 1.122804 H -0.313971 -2.425943 3.453548 H -5.658844 3.432762 -0.763653 H -4.662694 1.394120 2.629662 H 0.284441 -2.501198 1.045272 H -3.619493 3.559216 3.196846 Si -0.426180 1.100887 -0.982857 O 1.097100 1.312660 -1.533616 O 0.537322 2.252262 2.932136 H 0.254783 3.203171 2.880635 O -3.217761 2.082571 -4.078016 H -3.348856 3.046011 -3.885908 O -1.090805 -2.533004 -2.732923 H -1.639078 -3.167463 -3.227872 Y -1.638420 3.982164 -0.369294 O 0.222871 4.059220 -1.229095 C 1.967475 2.402050 -1.187435 C 1.477445 3.742647 -1.754531 H 2.048310 2.481026 -0.079188 H 2.965124 2.145516 -1.598639 H 1.392813 3.619425 -2.864969 C 2.496125 4.848888 -1.450741 H 3.492295 4.624845 -1.886223 H 2.146325 5.811605 -1.874107 H 2.609339 4.973616 -0.353016 Cl -1.166694 4.679414 2.115557 Cl -3.412619 4.581959 -2.226533 O -1.583870 6.360296 -0.464230 C -0.425070 7.206762 -0.269918 C -1.041940 7.088617 -1.611161 H 0.507318 6.659240 -0.051933 H -0.629902 8.095672 0.351560 H -0.532201 6.406996 -2.317998 C -1.953903 8.123457 -2.206803 H -1.382478 8.783883 -2.891782 H -2.752473 7.621839 -2.789357 H -2.424577 8.745182 -1.419766
(OH) $\mathbf{I}_{AB}$ (X = Br)	(OH) **B** (X = Br)
SCF Done: -4734.12547460 A.U. Si -6.428482 6.479224 1.185246 Si -7.814698 2.562155 1.024081 Si -6.927337 2.651492 -1.854297 Si -4.968665 5.132778 3.465618 Si -5.887557 0.148697 1.592289 Si -5.870013 5.348440 -1.704633 Si -3.885123 2.467162 2.342080 O -4.642329 3.504363 3.404912 O -7.283882 1.066111 1.537741 O -6.665286 5.842189 -0.324951 O -4.654042 1.017152 2.310465 O -8.045400 2.576981 -0.632754 O -6.808464 4.208409 -2.457644 O -4.997029 5.823444 1.888816 O -5.451388 2.234294 -1.241323 O -4.458528 4.591860 -1.195816 O -4.009123 3.258402 0.876867 H -7.565321 6.005866 2.035876 H -6.805137 3.589526 1.418074 H -9.145816 2.811491 1.649714 H -6.170828 -1.012660 2.491023 H -6.353462 7.964387 1.180408 H -6.350569 5.290884 4.020007 H -5.480984 -0.282493 0.224065 H -3.968253 5.867848 4.283653 Si -3.951255 2.891960 -0.806376 O -3.191827 1.375197 -0.997575 O -2.315510 2.170740 2.765881 H -1.834990 3.033956 2.841406 O -5.572670 6.577525 -2.755562	SCF Done: -4734.16098330 A.U. Si -4.913028 2.428458 0.456280 Si -3.125692 -1.369611 0.201961 Si -2.252953 -0.431341 -2.519623 Si -3.226442 2.401193 2.961568 Si -0.155490 -1.740653 1.140305 Si -3.375731 2.229790 -2.290767 Si -0.511802 1.249210 2.073598 O -1.892865 1.406100 2.995452 O -1.748723 -2.109547 0.787561 O -4.443643 1.916908 -1.050236 O -0.062340 -0.336148 2.033537 O -3.134978 -1.367155 -1.471967 O -3.177176 0.813966 -3.141360 O -3.573651 2.946696 1.383260 O -0.985310 0.233408 -1.700736 O -1.905009 2.630069 -1.597007 O -0.965160 1.807423 0.575202 H -5.464981 1.218982 1.151589 H -3.193296 0.022736 0.734238 H -4.295908 -2.193002 0.629959 H 0.345103 -2.840201 2.025857 H -5.948915 3.496178 0.394296 H -4.395383 1.570854 3.404490 H 0.647827 -1.627926 -0.110796 H -3.051446 3.585407 3.845146 Si -0.434469 1.700610 -1.047465 O 1.172832 1.090376 -0.993098 O 0.766569 2.084783 2.709787 H 0.514461 3.044473 2.761930 O -3.903500 3.388390 -3.338265

H	-5.032779	7.271560	-2.304290	H	-4.062382	4.218129	-2.818114
O	-7.461694	1.628722	-3.038341	O	-1.779254	-1.439717	-3.747156
H	-6.957863	1.695211	-3.868868	H	-1.345496	-0.965661	-4.478677
Y	-2.934661	5.512703	0.303843	Y	-1.581437	4.384114	-0.051059
O	-2.319503	3.673377	-0.998464	O	0.255607	3.359472	-1.125620
C	-1.811286	1.383319	-0.683248	C	2.112848	2.035869	-0.519179
C	-1.223938	2.749648	-1.108652	C	1.684329	3.428656	-1.035103
H	-1.663233	1.245097	0.414629	H	2.130949	2.046798	0.597582
H	-1.302193	0.549216	-1.212284	H	3.130133	1.770763	-0.882337
H	-0.940552	2.721528	-2.187488	H	2.066576	3.578702	-2.073990
C	-0.026758	3.164518	-0.267461	C	2.135208	4.579820	-0.149193
H	0.784304	2.414251	-0.377118	H	3.244635	4.622377	-0.116163
H	0.364030	4.153306	-0.572725	H	1.744153	5.544926	-0.525889
H	-0.303772	3.222522	0.804418	H	1.757774	4.446990	0.885509
Cl	-1.672363	5.221402	2.542791	Cl	-0.757932	4.764402	2.402874
Cl	-3.894771	7.825892	-0.388184	Cl	-3.955172	5.240359	-0.861960
O	-1.077361	6.220023	-0.753453	O	-0.775442	6.117853	-0.847904
C	-0.526144	7.486525	-1.447349	C	-1.685807	7.909969	-1.986536
C	-0.702145	6.247937	-2.195074	C	-0.608117	6.822676	-2.040485
H	0.463384	7.759680	-1.057884	H	-1.587063	8.517520	-1.069168
H	-1.290548	8.274466	-1.520772	H	-2.701900	7.478722	-2.062951
H	0.214151	5.655881	-2.373343	H	0.395703	7.323339	-2.055166
C	-1.797209	6.069885	-3.206607	C	-0.718729	5.907269	-3.267397
H	-1.425074	6.498717	-4.160347	H	-0.550932	6.461798	-4.213193
H	-2.054602	5.001026	-3.341237	H	0.028558	5.093244	-3.184876
H	-2.710075	6.622731	-2.913337	H	-1.723797	5.436424	-3.309167
Br	0.772706	8.741758	-3.893913	Br	-1.550157	9.272475	-3.520465
(OH) $\mathbf{I}_{BC}$ (X = Br)				(OH) **C** (X = Br)			
SCF Done: -4922.61352114 A.U.				SCF Done: -4922.61988085 A.U.			
Si	-4.445212	1.804532	0.807688	Si	-5.132784	1.893014	-0.253646
Si	-2.392627	-1.208831	2.655127	Si	-3.094602	-1.568251	0.811386
Si	-1.307092	-1.829478	-0.066574	Si	-1.783429	-1.277703	-1.907433
Si	-2.807113	3.018103	3.060151	Si	-3.654584	2.445903	2.374984
Si	0.528432	-0.894477	3.689228	Si	-0.248866	-1.467753	2.053959
Si	-2.796742	0.333646	-1.426965	Si	-3.296914	1.141830	-2.698599
Si	0.127848	2.117574	2.718570	Si	-0.691235	1.701264	1.952510
O	-1.319659	2.399556	3.490639	O	-2.181659	1.728514	2.694813
O	-1.092058	-1.311298	3.695641	O	-1.851521	-1.911271	1.869932
O	-3.878356	0.599427	-0.189403	O	-4.453963	1.033285	-1.505465
O	0.759794	0.686009	3.239146	O	-0.064224	0.179750	2.029735
O	-2.146045	-2.186919	1.315106	O	-2.675448	-2.037060	-0.740571
O	-2.294907	-1.254687	-1.273328	O	-2.741393	-0.413816	-2.954370
O	-3.145780	2.768285	1.391283	O	-3.883751	2.618486	0.677308
O	-0.212102	-0.620384	0.299852	O	-0.748363	-0.194572	-1.162459
O	-1.445285	1.292943	-1.114483	O	-2.002940	2.004031	-2.042693
O	-0.302621	1.984123	1.105850	O	-1.048590	2.070570	0.350301
H	-5.003284	1.097699	2.006362	H	-5.785596	0.883514	0.640966
H	-2.549983	0.206431	2.218865	H	-3.370349	-0.103836	0.845825
H	-3.590676	-1.729366	3.374375	H	-4.276692	-2.380318	1.220635
H	1.007377	-1.060248	5.097699	H	0.175140	-1.979544	3.394851
H	-5.477647	2.665778	0.177631	H	-6.088940	2.933347	-0.706833
H	-3.821873	2.207288	3.809571	H	-4.707525	1.484836	2.837185
H	1.286742	-1.778692	2.751758	H	0.580282	-2.057600	0.958640
H	-2.935657	4.463608	3.372542	H	-3.776606	3.780249	3.011037
Si	-0.085520	0.974610	-0.192509	Si	-0.683001	1.475726	-1.161561
O	1.407634	1.095605	-0.875048	O	0.834683	1.872891	-1.652784
O	1.297768	3.246774	2.954862	O	0.452238	2.698427	2.577037
H	0.935690	4.111134	2.608579	H	0.119270	3.635484	2.447683
O	-3.375379	0.510707	-2.950978	O	-3.794877	1.729670	-4.144011
H	-3.605092	1.475935	-3.041248	H	-4.012599	2.690580	-3.980789
O	-0.569941	-3.231993	-0.541482	O	-0.966414	-2.469194	-2.712060
H	-0.191151	-3.182366	-1.437252	H	-0.520234	-2.155000	-3.518575
O	0.192262	3.552791	-1.272911	O	-0.511493	4.303036	-1.447832
C	2.172358	2.308947	-0.818435	C	1.504378	3.052038	-1.173280
C	1.522532	3.427994	-1.650387	C	0.851117	4.341358	-1.705902
H	2.259395	2.649676	0.239374	H	1.482592	3.066548	-0.059266
H	3.187787	2.067513	-1.197511	H	2.561129	2.974649	-1.505162
H	1.577250	3.118756	-2.728161	H	1.022349	4.367083	-2.815593
C	2.298899	4.737626	-1.463647	C	1.525890	5.562911	-1.065569
H	3.371987	4.624757	-1.730654	H	2.626306	5.561258	-1.222962
H	1.871810	5.538275	-2.098610	H	1.124473	6.501261	-1.496917

H	2.226786	5.067699	-0.406144	H	1.316652	5.574567	0.024379
Y	-1.630234	3.969305	-0.384122	Y	-2.376441	4.261907	-0.527800
Cl	-3.710138	3.349759	-1.978531	Cl	-4.178592	4.234566	-2.518935
Cl	-0.635411	5.227805	1.777599	Cl	-1.302593	4.995352	1.845294
O	-1.799525	5.937733	-1.254645	O	-2.567811	6.576027	-0.771513
C	-0.971701	6.745804	-2.049407	C	-1.746832	7.675093	-1.208441
H	-0.239499	6.100984	-2.596021	H	-0.939975	7.179726	-1.788332
C	-1.788331	7.538854	-3.073529	C	-2.523857	8.629455	-2.109987
H	-1.131746	8.147708	-3.728259	H	-1.846329	9.404344	-2.521560
H	-2.365307	6.830285	-3.701127	H	-2.965652	8.057647	-2.950192
H	-2.504217	8.210139	-2.557711	H	-3.339407	9.114657	-1.540799
C	-0.193782	7.607889	-1.052110	C	-1.135549	8.289322	0.050326
H	0.334922	6.980671	-0.312557	H	-0.679156	7.508055	0.686089
H	-0.842637	8.344263	-0.542843	H	-1.867888	8.886599	0.621591
Br	1.282693	8.731891	-1.936573	Br	0.382803	9.565398	-0.413247
C	-3.381871	6.656481	0.020163	C	-3.762660	6.751382	0.146132
O	-3.443900	7.819027	-0.184627	O	-4.127944	7.880888	0.414796
O	-3.622555	5.581808	0.483285	O	-4.119944	5.579941	0.448186
(OH) $\mathbf{I}_{\mathbf{cD}}$ (X = Br)				(OH) **D** (X = Br)			
SCF Done: -4922.59997552 A.U.				SCF Done: -4922.61105475 A.U.			
Si	-4.276789	1.862354	-1.624208	Si	-4.297493	1.762713	-1.565485
Si	-1.858516	-1.552670	-1.007109	Si	-1.799076	-1.541122	-1.065017
Si	-0.326331	-0.576545	-3.392860	Si	-0.343441	-0.504121	-3.479927
Si	-3.067875	1.778757	1.181273	Si	-3.083006	1.707999	1.229435
Si	0.817870	-1.430034	0.605528	Si	0.904623	-1.387697	0.510411
Si	-2.095857	1.793209	-3.844645	Si	-2.148474	1.843363	-3.840309
Si	0.038222	1.597011	1.102697	Si	0.022607	1.606108	1.071048
O	-1.532981	1.219830	1.502411	O	-1.524696	1.193967	1.516633
O	-0.722696	-1.906427	0.158508	O	-0.614525	-1.910795	0.045730
O	-3.438273	1.348928	-2.968896	O	-3.426073	1.322501	-2.914469
O	0.894533	0.199744	0.920802	O	0.915605	0.241541	0.850148
O	-1.189219	-1.698350	-2.538867	O	-1.193373	-1.634895	-2.627329
O	-1.310412	0.397699	-4.312253	O	-1.333802	0.489831	-4.373377
O	-3.164784	2.406237	-0.425351	O	-3.224028	2.373513	-0.360536
O	0.464809	0.410443	-2.293442	O	0.457468	0.468910	-2.370488
O	-1.068038	2.559826	-2.743922	O	-1.088623	2.627272	-2.777254
O	-0.076192	2.341909	-0.402819	O	-0.161946	2.347228	-0.435903
H	-4.946398	0.649833	-1.056288	H	-4.869479	0.496013	-1.010688
H	-2.342113	-0.153852	-0.825868	H	-2.285186	-0.153222	-0.820169
H	-2.956428	-2.554928	-0.895552	H	-2.881284	-2.557703	-0.940199
H	1.136512	-2.178511	1.860887	H	1.244728	-2.140013	1.756881
H	-5.239477	2.950246	-1.927361	H	-5.351010	2.768486	-1.848015
H	-3.962119	0.576707	1.196314	H	-3.933999	0.475758	1.226636
H	1.790365	-1.745370	-0.484846	H	1.893500	-1.642612	-0.580029
H	-3.522210	2.817304	2.138566	H	-3.560284	2.703803	2.219753
Si	0.336702	2.043070	-1.983419	Si	0.308957	2.085030	-2.014103
O	1.766568	2.710449	-2.438167	O	1.733839	2.795502	-2.399695
O	0.851151	2.525151	2.181979	O	0.840482	2.565914	2.118342
H	0.373133	3.400704	2.223535	H	0.331859	3.418707	2.198650
O	-2.374927	2.676591	-5.194722	O	-2.526559	2.751877	-5.148814
H	-2.717189	3.560308	-4.881391	H	-2.915283	3.600433	-4.805444
O	0.720872	-1.420782	-4.350857	O	0.695888	-1.328024	-4.460552
H	1.173978	-0.872728	-5.016169	H	1.119282	-0.778976	-5.144407
O	0.127557	4.896009	-1.768495	O	0.061028	4.961111	-1.706213
C	2.298685	3.934650	-1.904669	C	2.239856	4.000640	-1.794496
C	1.407664	5.141380	-2.242220	C	1.366083	5.221655	-2.119316
H	2.388024	3.849524	-0.797325	H	2.285686	3.869559	-0.689272
H	3.314370	4.052232	-2.337268	H	3.271297	4.135689	-2.180225
H	1.383832	5.231851	-3.361107	H	1.379937	5.355999	-3.232255
C	1.990913	6.430384	-1.649468	C	1.924835	6.482809	-1.451096
H	3.019042	6.631001	-2.019798	H	2.970864	6.684239	-1.764931
H	1.352280	7.293774	-1.922207	H	1.315892	7.368955	-1.718781
H	2.013448	6.362298	-0.541623	H	1.897207	6.371888	-0.346930
Y	-1.725381	4.397755	-1.025298	Y	-1.744672	4.346965	-0.986028
Cl	-3.270031	4.754843	-3.191229	Cl	-3.482427	4.669289	-2.975470
Cl	-1.257941	4.589488	1.587692	Cl	-1.401140	4.545641	1.620321
O	-2.148727	6.768195	-0.768097	O	-2.215001	6.691788	-0.731452
C	-1.812057	8.124174	-1.220749	C	-1.793222	8.014076	-1.276638
H	-0.790173	8.298484	-0.838181	H	-0.796459	8.233737	-0.855994
C	-1.860848	8.171673	-2.739298	C	-1.771733	7.946596	-2.788715
H	-1.565183	9.184223	-3.076474	H	-1.406604	8.927896	-3.153681

H -1.165111 7.421792 -3.162913	H -1.079792 7.147933 -3.121853
H -2.881834 7.937526 -3.101757	H -2.779994 7.731251 -3.196709
C -2.789141 9.066379 -0.522745	C -2.870578 8.919705 -0.646850
H -2.677737 9.272169 0.547066	H -2.521644 9.428032 0.270694
H -3.484969 9.683737 -1.097737	H -3.282722 9.666279 -1.346386
Br -1.222798 11.141285 -0.805790	Br -0.466133 11.036657 -1.296125
C -3.475321 6.624549 -0.349411	C -3.507716 6.740563 -0.280106
O -4.114361 7.712839 -0.233557	O -3.963881 7.984876 -0.278678
O -3.810288 5.439406 -0.161089	O -4.079520 5.715839 0.044433
(OH) $\mathbf{I_{AB}}$ (X = I)	(OH) **B** (X = I)
SCF Done: -4732.19232771 A.U.	SCF Done: -4732.22327531 A.U.
Si -6.419276 6.480121 1.174449	Si -4.909492 2.430423 0.442252
Si -7.814665 2.572184 1.028596	Si -3.130232 -1.368499 0.217567
Si -6.933172 2.643138 -1.850160	Si -2.251338 -0.452703 -2.509116
Si -4.962070 5.137425 3.457406	Si -3.226801 2.409916 2.949649
Si -5.902904 0.151204 1.606866	Si -0.161595 -1.743449 1.154584
Si -5.865817 5.336673 -1.710085	Si -3.370055 2.211604 -2.301939
Si -3.886951 2.464523 2.344043	Si -0.510352 1.253829 2.071774
O -4.643338 3.506993 3.402015	O -1.892339 1.416373 2.991067
O -7.295099 1.075099 1.550944	O -1.756748 -2.110743 0.808600
O -6.660865 5.838883 -0.333727	O -4.440270 1.908902 -1.060820
O -4.662436 1.017727 2.314352	O -0.063415 -0.332081 2.036183
O -8.050839 2.576347 -0.627831	O -3.138246 -1.377923 -1.456295
O -6.807968 4.196785 -2.459760	O -3.171370 0.789808 -3.142367
O -4.990185 5.823300 1.879567	O -3.569009 2.950338 1.367796
O -5.458858 2.222363 -1.235254	O -0.984307 0.216418 -1.692594
O -4.457271 4.577114 -1.198813	O -1.900115 2.615227 -1.607924
O -4.001875 3.251713 0.875998	O -0.961032 1.808727 0.570824
H -7.557703 6.012687 2.026624	H -5.464998 1.226453 1.143965
H -6.794301 3.593118 1.410712	H -3.191085 0.028260 0.739148
H -9.141490 2.837627 1.656700	H -4.304563 -2.182880 0.651242
H -6.189359 -1.002819 2.514188	H 0.338295 -2.837219 2.047563
H -6.341888 7.965178 1.164506	H -5.942015 3.500933 0.373908
H -6.342259 5.302227 4.014546	H -4.396638 1.579453 3.389666
H -5.504176 -0.292346 0.240238	H 0.639205 -1.642477 -0.099131
H -3.957548 5.870521 4.272293	H -3.057472 3.596553 3.830962
Si -3.955667 2.875669 -0.804799	Si -0.431339 1.688461 -1.052012
O -3.204645 1.351915 -0.982362	O 1.175061 1.077365 -0.994507
O -2.319950 2.161480 2.772953	O 0.769337 2.088315 2.706663
H -1.835731 3.023296 2.842929	H 0.518091 3.048151 2.758452
O -5.564568 6.559508 -2.767768	O -3.895151 3.362365 -3.359193
H -5.027986 7.255956 -2.315712	H -4.055278 4.195921 -2.846183
O -7.471251 1.618316 -3.031033	O -1.776511 -1.471853 -3.727173
H -6.973871 1.688646 -3.865102	H -1.338175 -1.005065 -4.460644
Y -2.918195 5.499776 0.287306	Y -1.576482 4.371753 -0.063012
O -2.323331 3.646423 -1.017978	O 0.260146 3.347280 -1.138929
C -1.823738 1.358382 -0.670819	C 2.115633 2.023833 -0.523758
C -1.232203 2.716377 -1.116918	C 1.688910 3.415564 -1.044490
H -1.673273 1.234741 0.428562	H 2.133426 2.038345 0.592945
H -1.318917 0.514899 -1.189136	H 3.132800 1.756574 -0.885601
H -0.951344 2.671033 -2.195988	H 2.073863 3.562900 -2.082672
C -0.031444 3.139715 -0.284965	C 2.138998 4.567963 -0.159743
H 0.776070 2.383921 -0.382903	H 3.248400 4.608807 -0.123878
H 0.362810 4.122132 -0.606316	H 1.750490 5.533034 -0.539061
H -0.306245 3.217624 0.786330	H 1.758944 4.437732 0.874336
Cl -1.665170 5.205469 2.533411	Cl -0.760056 4.762942 2.391142
Cl -3.889745 7.811963 -0.409524	Cl -3.942982 5.228983 -0.891957
O -1.069151 6.195625 -0.760097	O -0.760944 6.109323 -0.850722
C -0.507821 7.544576 -1.490692	C -1.691779 7.914346 -1.928810
C -0.691913 6.266188 -2.174088	C -0.606385 6.836823 -2.032119
H 0.458607 7.803336 -1.041924	H -1.582201 8.495862 -0.995865
H -1.310373 8.295098 -1.513813	H -2.705892 7.476833 -1.999702
H 0.233322 5.689582 -2.370308	H 0.396994 7.337719 -2.045809
C -1.782419 6.057660 -3.191588	C -0.725690 5.936442 -3.269441
H -1.424010 6.445084 -4.166820	H -0.556952 6.493293 -4.213779
H -2.036049 4.983425 -3.282808	H 0.019294 5.119267 -3.194529
H -2.698645 6.613677 -2.914681	H -1.731291 5.466885 -3.310916
I 0.785243 9.099000 -3.859227	I -1.615540 9.486308 -3.556686
(OH) $\mathbf{I_{BC}}$ (X = I)	(OH) **C** (X = I)
SCF Done: -4920.67548184 A.U.	SCF Done: -4920.68146940 A.U.
Si -4.442451 1.808831 0.802911	Si -5.130304 1.895766 -0.255669

Si -2.400143 -1.209986 2.657137	Si -3.099548 -1.568240 0.808482
Si -1.309998 -1.833023 -0.062381	Si -1.785674 -1.279424 -1.908432
Si -2.803825 3.016541 3.059158	Si -3.653265 2.445462 2.374501
Si 0.520186 -0.901640 3.695435	Si -0.254719 -1.473572 2.053920
Si -2.793311 0.332759 -1.426804	Si -3.293803 1.143322 -2.699659
Si 0.130075 2.111350 2.723389	Si -0.690980 1.696115 1.954429
O -1.318378 2.395533 3.492974	O -2.181817 1.725710 2.695893
O -1.101695 -1.313194 3.700047	O -1.858132 -1.913619 1.868190
O -3.879264 0.601661 -0.193764	O -4.452437 1.035958 -1.507935
O 0.757268 0.677108 3.242120	O -0.066339 0.173611 2.030657
O -2.151920 -2.188700 1.317849	O -2.680095 -2.038325 -0.743103
O -2.294679 -1.256259 -1.270737	O -2.740695 -0.413099 -2.956070
O -3.138869 2.765110 1.389642	O -3.880263 2.617895 0.676571
O -0.213219 -0.625914 0.306257	O -0.750087 -0.198552 -1.160687
O -1.441771 1.289860 -1.109124	O -1.999179 2.002672 -2.041758
O -0.298314 1.981339 1.109472	O -1.047228 2.067185 0.352327
H -5.007538 1.105110 2.000034	H -5.785455 0.886812 0.637846
H -2.555311 0.205236 2.219720	H -3.371973 -0.103194 0.842357
H -3.600162 -1.728879 3.374227	H -4.283781 -2.377570 1.216893
H 0.996183 -1.066108 5.105017	H 0.166835 -1.986902 3.394987
H -5.467233 2.676415 0.169115	H -6.084106 2.938381 -0.708538
H -3.822098 2.208987 3.807198	H -4.708602 1.486937 2.836396
H 1.277011 -1.790066 2.760789	H 0.574165 -2.064618 0.959074
H -2.928859 4.463030 3.368309	H -3.772301 3.780743 3.009235
Si -0.083338 0.968330 -0.186570	Si -0.681396 1.471553 -1.159253
O 1.409859 1.087980 -0.868966	O 0.837792 1.865665 -1.648393
O 1.302564 3.236900 2.963315	O 0.453439 2.691325 2.580156
H 0.944099 4.102673 2.616687	H 0.122476 3.629165 2.450748
O -3.365779 0.510901 -2.952977	O -3.789327 1.733568 -4.144944
H -3.590817 1.477029 -3.045345	H -4.004994 2.694825 -3.981172
O -0.574453 -3.236663 -0.536121	O -0.969240 -2.471322 -2.712984
H -0.195358 -3.188426 -1.431839	H -0.521893 -2.157251 -3.518898
O 0.195807 3.548417 -1.273996	O -0.506292 4.297919 -1.446302
C 2.174182 2.301953 -0.817102	C 1.508129 3.044830 -1.169765
C 1.524443 3.416332 -1.654783	C 0.856274 4.333621 -1.704926
H 2.260481 2.647531 0.239170	H 1.485432 3.060781 -0.055799
H 3.189863 2.059069 -1.194517	H 2.565077 2.966115 -1.500656
H 1.574610 3.098417 -2.730216	H 1.027130 4.356417 -2.814713
C 2.302023 4.726627 -1.481110	C 1.531254 5.556479 -1.067844
H 3.373963 4.613732 -1.752284	H 2.631342 5.556767 -1.227175
H 1.869704 5.519534 -2.122249	H 1.127226 6.492264 -1.502469
H 2.233036 5.065719 -0.426255	H 1.323264 5.570381 0.022335
Y -1.622083 3.966775 -0.378947	Y -2.370139 4.261078 -0.524480
Cl -3.692938 3.353687 -1.986444	Cl -4.170048 4.238538 -2.517994
Cl -0.619186 5.224093 1.778830	Cl -1.291505 4.995551 1.845712
O -1.792477 5.944327 -1.246719	O -2.565947 6.576738 -0.764103
C -0.976704 6.762299 -2.046136	C -1.754172 7.681668 -1.209698
H -0.237444 6.122692 -2.588707	H -0.948047 7.186070 -1.790713
C -1.812790 7.532569 -3.072161	C -2.549270 8.618517 -2.114850
H -1.178001 8.149118 -3.740949	H -1.889418 9.397474 -2.547204
H -2.379707 6.805262 -3.687364	H -2.993314 8.028892 -2.941465
H -2.539889 8.192888 -2.558256	H -3.365554 9.100692 -1.544163
C -0.216144 7.629716 -1.038334	C -1.148693 8.297322 0.052330
H 0.320903 7.001434 -0.304975	H -0.677861 7.516094 0.677968
H -0.878545 8.347037 -0.519124	H -1.891401 8.871934 0.634112
I 1.396493 8.920529 -1.954666	I 0.498968 9.741462 -0.403030
C -3.371164 6.641362 0.008481	C -3.765154 6.747131 0.150561
O -3.456971 7.803153 -0.195482	O -4.138339 7.874675 0.415969
O -3.602614 5.567373 0.481275	O -4.115936 5.574128 0.453630
(OH) $\mathbf{I}_{\mathbf{CD}}$ (X = I)	(OH) **D** (X = I)
SCF Done: -4920.66302875 A.U.	SCF Done: -4920.67718415 A.U.
Si -4.276007 1.854130 -1.615936	Si -4.283075 1.801692 -1.555015
Si -1.854066 -1.554118 -1.016794	Si -1.832815 -1.541616 -1.057611
Si -0.328808 -0.568526 -3.404793	Si -0.374438 -0.528452 -3.483276
Si -3.064438 1.771712 1.188349	Si -3.054208 1.735194 1.236365
Si 0.825322 -1.433078 0.589118	Si 0.882258 -1.419909 0.500241
Si -2.101194 1.800274 -3.844935	Si -2.146301 1.845061 -3.843652
Si 0.040464 1.592511 1.096876	Si 0.046921 1.588659 1.060054
O -1.528013 1.214014 1.505339	O -1.502138 1.202441 1.522942
O -0.714196 -1.913798 0.143172	O -0.646982 -1.923570 0.047335
O -3.436455 1.347679 -2.962546	O -3.428471 1.349447 -2.910161

O 0.896845 0.196863 0.905009	O 0.916880 0.210857 0.832257
O -1.190078 -1.691976 -2.551524	O -1.236076 -1.643808 -2.622688
O -1.313753 0.408289 -4.320313	O -1.355086 0.477113 -4.374333
O -3.165621 2.401851 -0.416985	O -3.189248 2.391295 -0.357975
O 0.464440 0.416229 -2.304476	O 0.445701 0.437109 -2.380889
O -1.068705 2.568000 -2.749209	O -1.071191 2.616870 -2.786832
O -0.085087 2.340690 -0.406707	O -0.145924 2.328511 -0.447135
H -4.936733 0.636089 -1.049397	H -4.876472 0.546763 -0.996580
H -2.336441 -0.156187 -0.825906	H -2.301296 -0.147487 -0.811682
H -2.951601 -2.556868 -0.906739	H -2.926622 -2.544715 -0.926344
H 1.147673 -2.181430 1.843556	H 1.219988 -2.170945 1.747929
H -5.247221 2.935640 -1.914533	H -5.315321 2.831215 -1.831180
H -3.957691 0.569030 1.204133	H -3.925276 0.517365 1.246081
H 1.797646 -1.743894 -0.502646	H 1.860276 -1.691930 -0.595722
H -3.516563 2.809212 2.147821	H -3.509736 2.749396 2.218517
Si 0.333159 2.046773 -1.987402	Si 0.318776 2.054685 -2.025537
O 1.763303 2.720799 -2.430642	O 1.752586 2.749702 -2.407272
O 0.860583 2.518820 2.172242	O 0.891598 2.539372 2.093949
H 0.382287 3.394036 2.219365	H 0.399128 3.402022 2.174396
O -2.390906 2.684774 -5.192132	O -2.515155 2.753508 -5.154454
H -2.737171 3.565398 -4.875339	H -2.884324 3.612180 -4.814964
O 0.717115 -1.410355 -4.366178	O 0.648245 -1.369293 -4.466498
H 1.165955 -0.861630 -5.033829	H 1.067999 -0.830958 -5.161036
O 0.120675 4.907885 -1.760586	O 0.110866 4.941981 -1.716180
C 2.291134 3.937838 -1.876735	C 2.273226 3.936536 -1.779375
C 1.408826 5.151227 -2.213657	C 1.428252 5.178797 -2.101295
H 2.365129 3.841099 -0.769211	H 2.300701 3.791187 -0.675301
H 3.313010 4.057231 -2.293922	H 3.312687 4.056525 -2.148318
H 1.401139 5.253889 -3.331678	H 1.466376 5.330589 -3.211364
C 1.991194 6.430331 -1.598745	C 2.000648 6.416916 -1.401770
H 3.025541 6.628969 -1.952321	H 3.052166 6.610792 -1.701660
H 1.362187 7.300887 -1.871071	H 1.403113 7.313925 -1.657940
H 1.997834 6.349884 -0.491503	H 1.959931 6.283762 -0.300437
Y -1.728175 4.396270 -1.013556	Y -1.700101 4.347296 -0.988454
Cl -3.288742 4.744873 -3.171828	Cl -3.418537 4.707273 -2.991941
Cl -1.251643 4.583948 1.597179	Cl -1.306838 4.564000 1.610039
O -2.146026 6.772523 -0.760426	O -2.165756 6.733563 -0.731690
C -1.811815 8.113581 -1.253590	C -1.845252 8.077660 -1.283182
H -0.774975 8.273766 -0.905679	H -0.871495 8.372732 -0.852334
C -1.903227 8.123732 -2.771403	C -1.799406 7.998930 -2.794038
H -1.591550 9.115157 -3.154162	H -1.508686 8.998684 -3.175525
H -1.241663 7.341619 -3.191409	H -1.045269 7.251709 -3.111002
H -2.940167 7.908458 -3.097951	H -2.783246 7.702032 -3.209416
C -2.755926 9.081907 -0.549036	C -2.999458 8.903757 -0.673764
H -2.645500 9.268274 0.524544	H -2.700353 9.458425 0.234936
H -3.465263 9.694086 -1.112547	H -3.465354 9.601899 -1.389838
I -1.101141 11.362405 -0.815376	I -0.744840 11.556229 -1.301877
C -3.478054 6.629875 -0.346607	C -3.459383 6.689571 -0.291320
O -4.123531 7.713633 -0.250072	O -4.012562 7.892128 -0.295753
O -3.803511 5.443431 -0.144925	O -3.954988 5.622277 0.028277
Model B1:	
Y	**Y-PO**
SCF Done: -4108.80580386 A.U.	SCF Done: -4301.83145350 A.U.
Si 3.586538 -1.379836 -0.187118	Si 4.032714 -0.578923 -0.597347
Si 1.884069 2.406691 -0.593271	Si 0.763152 2.496303 -0.647563
Si -0.451775 1.276858 -2.265654	Si -0.113791 -0.305592 -1.921163
Si 1.701880 -2.906378 1.815334	Si 4.610315 -2.061898 2.151424
Si 2.134140 1.264377 2.300394	Si 1.037077 2.083875 2.425849
Si 1.033677 -1.348946 -2.068792	Si 2.043941 -2.479503 -2.058281
Si -0.322886 -0.676226 2.664892	Si 1.860217 -1.012475 2.813247
O 0.325939 -2.183870 2.426146	O 3.420279 -1.455291 3.169434
O 1.998042 1.268439 0.624052	O 0.307018 2.114481 0.910203
O 2.574448 -1.197092 -1.506454	O 3.482589 -1.888981 -1.496493
O 0.849637 0.448919 2.978033	O 1.798453 0.632609 2.683047
O 0.353796 2.336910 -1.287502	O 0.353799 1.250772 -1.679670
O 0.577313 0.088692 -2.799412	O 1.111776 -1.193925 -2.609615
O 2.711052 -1.720134 1.195211	O 4.772574 -1.098808 0.794534
O -1.654582 0.493319 -1.330473	O -0.455739 -1.065545 -0.442067
O 0.004434 -1.587168 -0.765254	O 1.164750 -3.209910 -0.826406
O -1.139573 -0.220667 1.274897	O 1.566269 -1.666406 1.296903
H 4.346744 -0.118582 0.031980	H 2.879802 0.316953 -0.271987

H 2.909069 2.080669 -1.628125 H 0.939973 -2.457887 -3.041818 H 2.030743 3.781196 -0.025900 H 3.414276 0.600848 2.678606 H 4.494130 -2.532724 -0.487854 H 2.409250 -3.577604 2.947580 H 2.074730 2.681440 2.781037 H 1.316048 -3.875536 0.744010 H -1.141626 1.977094 -3.369322 H -1.270420 -0.713568 3.798821 Si -1.376501 -0.846953 -0.221281 O -2.776677 -1.632099 -0.473488 Y -3.663593 -0.497500 -2.039085 Cl -2.808086 -1.149420 -4.280194 Cl -5.797811 0.715728 -1.656497	H 2.239468 2.729202 -0.721411 H 2.284678 -3.457136 -3.138950 H -0.005875 3.696093 -1.098522 H 2.107048 3.132865 2.442139 H 5.066950 0.124749 -1.410534 H 5.897158 -2.000217 2.902125 H -0.020117 2.334948 3.442433 H 4.258708 -3.455501 1.732512 H -1.315430 -0.341673 -2.785224 H 0.924504 -1.524534 3.838723 Si 0.392556 -2.362892 0.370907 O -0.869583 -2.984310 1.162696 Y -2.346082 -1.413227 0.974155 Cl -4.668945 -2.244407 0.498592 Cl -1.969112 0.044130 2.975833 O -2.843406 0.458011 -0.408177 C -4.077548 0.859710 -1.074160 C -3.636166 1.578531 0.138609 H -4.881897 0.106313 -1.000199 H -3.902699 1.315315 -2.064468 H -4.136696 1.301942 1.085877 C -2.939249 2.906502 0.124145 H -3.656056 3.711140 0.387575 H -2.122333 2.901411 0.873221 H -2.507635 3.124097 -0.872320
$\mathbf{I}_{AB}$ (X = Br)	**B** (X = Br)
SCF Done: -4315.36767604 A.U. Si 3.806360 -0.248905 -0.015843 Si 0.443047 2.471177 -0.426535 Si -0.131830 -0.296664 -1.899780 Si 4.099722 -1.947617 2.626222 Si 0.299813 1.975472 2.683262 Si 2.175816 -2.268340 -1.792384 Si 1.266185 -1.034334 3.100813 O 2.826038 -1.417417 3.569602 O -0.036801 1.860877 1.044234 O 3.459076 -1.485637 -1.096248 O 1.108591 0.604582 3.187143 O 0.339268 1.243270 -1.561669 O 1.166261 -1.145472 -2.519103 O 4.441611 -0.873719 1.389729 O -0.623378 -1.107238 -0.498785 O 1.262002 -3.073361 -0.645478 O 1.197107 -1.518531 1.496862 H 2.578853 0.548683 0.270306 H 1.870436 2.926674 -0.369544 H 2.683278 -3.228832 -2.797056 H -0.472129 3.566178 -0.859738 H 1.262439 3.109707 2.881585 H 4.879696 0.585310 -0.636306 H 5.305548 -1.991760 3.507873 H -0.966157 2.162232 3.436332 H 3.796808 -3.295194 2.043108 H -1.240274 -0.303001 -2.879744 H 0.309342 -1.755038 3.967422 Si 0.225518 -2.316738 0.418960 O -1.029128 -3.114927 1.026726 Y -2.683097 -1.700617 0.800171 Cl -4.750929 -3.097959 0.536086 O -3.383434 0.097243 -0.389706 C -4.264303 1.225459 0.224710 C -3.049794 1.546804 -0.507925 H -4.243893 1.221125 1.324799 H -5.240663 1.286996 -0.277033 H -2.185932 1.812767 0.126198 C -3.096673 2.132002 -1.889010 H -3.301660 3.216098 -1.755121 H -2.140716 1.999577 -2.432978 H -3.922380 1.684362 -2.477044 Br -4.491709 4.270133 0.687262 Cl -2.364254 -0.437168 2.952819	SCF Done: -4315.41301864 A.U. Si -3.167331 1.684007 -0.835650 Si -3.388796 -1.610544 2.104490 Si -1.035638 -2.728056 0.371221 Si -0.603344 3.517461 -0.560248 Si -2.935421 1.152828 3.668254 Si -1.525384 -0.787783 -1.913937 Si -0.346994 1.982106 2.048345 O -0.484762 3.349088 1.099482 O -2.933818 -0.441031 3.194831 O -2.774041 0.275739 -1.641999 O -1.599294 1.980547 3.138552 O -2.086362 -2.539082 1.644190 O -1.789593 -2.185229 -1.028586 O -2.055494 2.889796 -1.114052 O 0.346285 -1.825059 0.583350 O -0.068804 -0.128634 -1.446806 O -0.537418 0.654036 1.052944 H -3.300982 1.428435 0.630929 H -4.018911 -0.978033 0.901311 H -1.503971 -1.116037 -3.360264 H -4.346252 -2.524083 2.804257 H -4.167931 1.824804 3.133544 H -4.467928 2.141695 -1.417342 H -0.626519 4.983447 -0.853402 H -2.920994 1.176375 5.163918 H 0.526686 2.823385 -1.247182 H -0.695366 -4.163722 0.252504 H 0.939897 2.009159 2.777124 Si 0.557695 -0.218703 0.113680 O 2.065624 0.302463 0.260615 Y 3.513045 0.468913 1.835107 Cl 3.961482 2.935239 2.263660 Cl 5.518286 -0.995115 1.303085 O 2.524908 -0.378221 3.441572 C 1.773879 -1.355227 4.100435 H 2.161256 -1.499787 5.141095 C 0.293304 -0.968968 4.168307 H -0.300720 -1.701024 4.750701 H 0.194686 0.027001 4.645435 H -0.137386 -0.917976 3.149636 C 2.038259 -2.630539 3.292754 H 3.109951 -2.900513 3.300150 H 1.657715 -2.524295 2.259733 Br 1.079035 -4.298138 4.013854

$\mathbf{I_{BC}}$ (X = Br)			
SCF Done: -4503.88257175 A.U.			
Si	-2.668107	1.776691	-1.718882
Si	-5.592503	-0.625238	0.377447
Si	-3.159918	-2.625402	0.439989
Si	-0.392881	2.904849	0.066238
Si	-5.013201	2.186077	1.956098
Si	-1.473997	-1.152751	-1.615323
Si	-1.933958	1.832831	2.418259
O	-1.339297	3.045759	1.450111
O	-5.450570	0.694000	1.366968
O	-2.105542	0.269440	-2.179370
O	-3.545128	2.143509	2.727906
O	-4.579301	-1.860307	0.849420
O	-2.720340	-2.156807	-1.107988
O	-1.450020	2.796955	-1.243846
O	-1.932447	-2.238229	1.489718
O	-0.464456	-0.904241	-0.312092
O	-1.861655	0.418284	1.541465
H	-3.660094	1.602159	-0.612471
H	-5.308935	-0.245534	-1.044062
H	-0.730817	-1.800409	-2.721828
H	-6.993954	-1.132893	0.530168
H	-4.998071	3.177370	0.830557
H	-3.312674	2.375344	-2.927709
H	0.383367	4.163074	-0.103582
H	-6.033506	2.565181	2.984823
H	0.426193	1.667080	0.091744
H	-3.405044	-4.088408	0.482779
H	-1.255883	1.745483	3.729449
Si	-0.891778	-0.925133	1.324852
O	0.393844	-0.982915	2.284853
Y	2.325747	-0.137356	2.573732
Cl	1.735150	2.343064	2.725777
Cl	3.623030	-0.744058	4.672923
O	3.340519	0.052627	0.674859
C	3.313840	0.990626	-0.381280
H	2.847688	1.933775	-0.005000
C	4.724641	1.292906	-0.886972
H	4.700682	2.030847	-1.714913
H	5.333593	1.708508	-0.059067
H	5.210720	0.363211	-1.247925
C	2.386260	0.387689	-1.440558
H	1.427208	0.070611	-0.990734
H	2.857529	-0.448362	-1.990065
Br	1.847422	1.732995	-2.874592
C	3.736615	-2.034549	0.444125
O	4.257034	-2.158748	-0.608564
O	3.270646	-2.325502	1.509452

C (X = Br)			
SCF Done: -4503.89246315 A.U.			
Si	-2.722287	1.917598	-1.694202
Si	-5.536218	-0.585272	0.402486
Si	-3.169933	-2.645305	0.315454
Si	-0.325746	2.856353	0.019772
Si	-4.959682	2.125025	2.133092
Si	-1.585641	-1.060662	-1.732895
Si	-1.850539	1.784829	2.384909
O	-1.242914	2.995886	1.422580
O	-5.356047	0.637427	1.505911
O	-2.298535	0.370068	-2.162014
O	-3.429599	2.145500	2.777049
O	-4.580848	-1.896663	0.782890
O	-2.773146	-2.136855	-1.231738
O	-1.407214	2.840687	-1.276469
O	-1.917656	-2.270576	1.342709
O	-0.522236	-0.867026	-0.460931
O	-1.872532	0.388122	1.474915
H	-3.680440	1.834025	-0.547793
H	-5.208308	-0.100844	-0.975935
H	-0.877685	-1.613678	-2.910282
H	-6.958365	-1.047732	0.492554
H	-5.095094	3.166750	1.062148
H	-3.364830	2.558492	-2.882694
H	0.508443	4.078952	-0.136906
H	-5.906499	2.395496	3.261048
H	0.428324	1.578488	-0.013860
H	-3.405592	-4.109550	0.330811
H	-1.103186	1.637045	3.653911
Si	-0.902194	-0.941023	1.183736
O	0.410542	-1.006685	2.108596
Y	2.259323	-0.226470	2.755751
Cl	1.958188	2.307326	2.464740
Cl	2.667906	-0.566858	5.225972
O	3.377170	0.027233	0.659297
C	3.277241	0.819148	-0.551698
H	2.710554	1.707714	-0.204567
C	4.652253	1.233314	-1.060648
H	4.541127	1.899205	-1.940014
H	5.193362	1.787839	-0.268335
H	5.242054	0.341655	-1.348158
C	2.416388	0.032116	-1.537210
H	1.509754	-0.367992	-1.044862
H	2.978442	-0.764556	-2.055750
Br	1.688364	1.244846	-2.991350
C	3.962554	-1.328681	0.691855
O	4.502363	-1.787292	-0.295643
O	3.734376	-1.762185	1.873218

$\mathbf{I_{CD}}$ (X = Br)			
SCF Done: -4503.86997219 A.U.			
Si	-2.357169	1.640819	-2.094795
Si	-5.114242	-0.515941	-0.129070
Si	-2.884792	-2.546830	0.547517
Si	-0.595759	3.406208	-0.042598
Si	-4.253289	2.017521	1.545079
Si	-1.133363	-1.272523	-1.490191
Si	-1.296491	2.007124	2.522529
O	-0.918110	3.345969	1.603521
O	-4.283606	0.844630	0.356566
O	-2.126818	0.013017	-1.810754
O	-2.957694	1.821068	2.568584
O	-4.421367	-1.906184	0.482281
O	-2.163412	-2.497964	-0.958487
O	-1.799946	2.561646	-0.822408
O	-1.961228	-1.649252	1.602276
O	-0.086015	-0.964555	-0.221078
O	-0.614173	0.703491	1.777382
H	-3.836363	1.847869	-2.167792
H	-5.119033	-0.546327	-1.622066
H	-0.394542	-1.763595	-2.672200

D (X = Br)			
SCF Done: -4503.88280147 A.U.			
Si	-2.369493	1.223380	-2.168695
Si	-4.820328	-1.005105	0.151145
Si	-2.357765	-2.369360	1.364124
Si	-0.703617	3.286457	-0.390469
Si	-4.475645	1.969138	1.151808
Si	-0.715516	-1.135618	-0.823723
Si	-1.728737	2.766222	2.404930
O	-1.330498	3.743386	1.133640
O	-4.178983	0.512743	0.390725
O	-1.831228	-0.299509	-1.699968
O	-3.323326	2.280316	2.308609
O	-3.978061	-2.137598	1.043109
O	-1.491752	-2.418095	-0.069488
O	-1.943220	2.343515	-1.011540
O	-1.796580	-1.064868	2.241914
O	-0.020638	-0.208563	0.391132
O	-0.743130	1.429329	2.448816
H	-3.865304	1.165068	-2.170870
H	-4.737825	-1.329415	-1.304732
H	0.354272	-1.672598	-1.695681

H -6.509104 -0.466615 0.423308	H -6.239642 -1.037582 0.639378
H -4.200236 3.351946 0.872598	H -4.514962 3.050958 0.123340
H -1.710383 2.054894 -3.374580	H -1.860291 1.536984 -3.530785
H -0.675355 4.850121 -0.433604	H -0.537260 4.569264 -1.124187
H -5.490497 1.878675 2.383796	H -5.787653 1.857890 1.874887
H 0.748691 2.835539 -0.326395	H 0.532791 2.542301 -0.042535
H -3.022961 -3.953191 0.999063	H -2.233042 -3.647071 2.096172
H -0.826271 2.190078 3.912523	H -1.566810 3.507282 3.681165
Si -0.471620 -0.905924 1.416718	Si -0.424004 -0.129463 2.028866
O 0.666792 -1.598859 2.340659	O 0.812825 -0.717951 2.918314
Y 2.506316 -1.045617 3.165961	Y 2.098689 -2.324277 3.062958
Cl 2.481531 1.384711 3.855446	Cl 3.808364 -2.198125 4.900875
Cl 3.042964 -2.491105 5.155044	Cl 0.737586 -4.417970 2.891872
O 2.909184 -0.159452 0.834025	O 3.130313 0.114796 0.607081
C 2.610486 0.653133 -0.358676	C 2.846814 0.977141 -0.575315
H 1.531979 0.867864 -0.277464	H 1.773671 1.242379 -0.497313
C 3.455662 1.912352 -0.309273	C 3.717671 2.207343 -0.551445
H 3.178581 2.563841 -1.160859	H 3.429897 2.823451 -1.428231
H 3.266676 2.448851 0.640838	H 3.526431 2.798481 0.365727
H 4.535787 1.665896 -0.376309	H 4.795746 1.949584 -0.606754
C 2.863949 -0.261880 -1.548614	C 3.067554 -0.008471 -1.734844
H 2.140108 -1.056907 -1.758183	H 2.262220 0.069463 -2.490995
H 3.571654 0.014192 -2.336405	H 4.063186 0.083366 -2.216422
Br 1.203279 1.152250 -3.066213	Br 0.963767 2.356740 -3.051534
C 3.738477 -1.217855 0.569583	C 3.069477 -1.146165 0.228339
O 4.056454 -1.381789 -0.646801	O 3.015350 -1.322236 -1.082014
O 4.041836 -1.892357 1.589628	O 3.072750 -2.101382 1.030059
I_{AB} (X = I)	**B** (X = I)
SCF Done: -4313.43480474 A.U.	SCF Done: -4313.47550769 A.U.
Si 3.854570 -0.341206 -0.052251	Si -3.168501 1.697573 -0.844570
Si 0.481920 2.478138 -0.360110	Si -3.395517 -1.603516 2.092373
Si -0.108035 -0.275081 -1.852124	Si -1.047238 -2.724620 0.356645
Si 4.169925 -1.996349 2.618891	Si -0.597363 3.519585 -0.563196
Si 0.394411 1.962941 2.719684	Si -2.942173 1.153055 3.661387
Si 2.151059 -2.312732 -1.794321	Si -1.533034 -0.776924 -1.922380
Si 1.344625 -1.067938 3.096277	Si -0.351139 1.982674 2.047690
O 2.899445 -1.463220 3.566641	O -0.484366 3.348623 1.096749
O -0.063135 1.905724 1.104938	O -2.935670 -0.441528 3.189187
O 3.473627 -1.600480 -1.094382	O -2.781083 0.287335 -1.650525
O 1.215681 0.576380 3.141345	O -1.605812 1.983047 3.135271
O 0.366411 1.264021 -1.504524	O -2.096970 -2.537728 1.631338
O 1.183836 -1.126835 -2.479857	O -1.800576 -2.176038 -1.040789
O 4.490167 -0.935412 1.365661	O -2.050200 2.897606 -1.121629
O -0.584375 -1.083473 -0.447870	O 0.336491 -1.825729 0.574736
O 1.218995 -3.110680 -0.656717	O -0.077371 -0.120568 -1.449271
O 1.260569 -1.582722 1.503633	O -0.540995 0.652880 1.054969
H 2.642234 0.486134 0.217517	H -3.303958 1.442421 0.621952
H 1.918707 2.894256 -0.263694	H -4.018758 -0.961859 0.890588
H 2.607211 -3.267877 -2.828088	H -1.508300 -1.102037 -3.369310
H -0.386769 3.603252 -0.816625	H -4.359786 -2.514479 2.785940
H 1.384557 3.080926 2.874147	H -4.174205 1.822216 3.122088
H 4.936222 0.459281 -0.702094	H -4.466412 2.161296 -1.427344
H 5.383090 -2.017706 3.490926	H -0.614505 4.985957 -0.854698
H -0.814278 2.161728 3.559489	H -2.932303 1.177990 5.156991
H 3.871719 -3.353642 2.057344	H 0.532144 2.822157 -1.247460
H -1.220477 -0.267038 -2.826754	H -0.710262 -4.160685 0.233173
H 0.375979 -1.748756 3.981738	H 0.933470 2.010006 2.780471
Si 0.233489 -2.333384 0.440982	Si 0.550322 -0.218310 0.110169
O -1.040567 -3.080499 1.070472	O 2.058912 0.301912 0.254483
Y -2.645538 -1.602329 0.847745	Y 3.501645 0.467266 1.831531
Cl -4.753508 -2.930847 0.560554	Cl 4.007253 2.928482 2.222257
O -3.254618 0.185657 -0.387427	Cl 5.461170 -1.071493 1.344575
C -4.384487 1.202660 0.095834	O 2.486442 -0.332740 3.447862
C -3.122718 1.650193 -0.485647	C 1.774759 -1.334790 4.114388
H -4.505343 1.181661 1.188894	H 2.176395 -1.462377 5.151469
H -5.278632 1.093874 -0.532439	C 0.283916 -0.990276 4.190646
H -2.380262 2.040903 0.234883	H -0.291687 -1.732867 4.778868
C -3.061737 2.215162 -1.877180	H 0.162493 0.004083 4.666178
H -3.374523 3.278522 -1.817013	H -0.152778 -0.947400 3.173948
H -2.039002 2.159990 -2.299334	C 2.082075 -2.595866 3.297671
H -3.765899 1.682229 -2.546538	H 3.168699 -2.793188 3.254509

I -5.585693 4.165213 0.463161	H 1.649379 -2.521545 2.281521
Cl -2.305173 -0.342380 2.999428	I 1.217933 -4.508874 4.129144
I_{BC} (X = I)	**C** (X = I)
SCF Done: -4501.94423759 A.U.	SCF Done: -4501.95372622 A.U.
Si -2.680725 1.751944 -1.714077	Si -2.776249 1.904659 -1.693610
Si -5.613371 -0.640929 0.398226	Si -5.573335 -0.589601 0.448301
Si -3.169694 -2.628976 0.460311	Si -3.195933 -2.635540 0.313131
Si -0.417050 2.927531 0.069706	Si -0.363395 2.876261 -0.009124
Si -5.020880 2.179561 1.955649	Si -4.945912 2.128271 2.154199
Si -1.471740 -1.170293 -1.597009	Si -1.633564 -1.064064 -1.766319
Si -1.943886 1.829865 2.421212	Si -1.837826 1.766995 2.369795
O -1.347453 3.051032 1.465120	O -1.250092 2.993264 1.414182
O -5.461999 0.683679 1.379265	O -5.375310 0.648446 1.530813
O -2.087641 0.255148 -2.170749	O -2.327702 0.375503 -2.198537
O -3.555156 2.137630 2.732718	O -3.412285 2.116037 2.789958
O -4.594882 -1.873177 0.866035	O -4.594227 -1.886796 0.816659
O -2.728880 -2.158724 -1.086582	O -2.831308 -2.115143 -1.237502
O -1.484087 2.792279 -1.228511	O -1.472266 2.845308 -1.280800
O -1.946187 -2.232725 1.511006	O -1.918538 -2.272943 1.312826
O -0.459854 -0.920074 -0.295633	O -0.544569 -0.873045 -0.515147
O -1.869726 0.425106 1.528730	O -1.864788 0.385395 1.436968
H -3.679290 1.560620 -0.616742	H -3.714316 1.781069 -0.534816
H -5.344730 -0.268180 -1.028077	H -5.289969 -0.117963 -0.944683
H -0.734422 -1.832139 -2.699191	H -0.960534 -1.641223 -2.952412
H -7.012620 -1.149043 0.567918	H -6.987909 -1.063791 0.584028
H -4.997476 3.160173 0.820985	H -5.066077 3.171418 1.082898
H -3.324143 2.341897 -2.927777	H -3.449516 2.554919 -2.859793
H 0.325964 4.204918 -0.105757	H 0.443272 4.116427 -0.174674
H -6.042596 2.572376 2.977670	H -5.880895 2.418259 3.287054
H 0.436983 1.711674 0.081371	H 0.423086 1.617228 -0.072991
H -3.406340 -4.093333 0.504370	H -3.435597 -4.099301 0.322706
H -1.264470 1.730080 3.730906	H -1.073093 1.603369 3.626215
Si -0.901413 -0.924189 1.337450	Si -0.901299 -0.946778 1.134937
O 0.372869 -0.971762 2.312441	O 0.420255 -1.016343 2.046116
Y 2.312689 -0.136077 2.563334	Y 2.243459 -0.226228 2.748559
Cl 1.748008 2.350233 2.712238	Cl 1.941819 2.304982 2.438182
Cl 3.636629 -0.737284 4.646298	Cl 2.577915 -0.556287 5.231897
O 3.308164 0.040504 0.649382	O 3.397971 0.024028 0.675019
C 3.345991 0.996534 -0.390991	C 3.324738 0.819309 -0.537911
H 2.902914 1.946967 -0.006082	H 2.750444 1.705906 -0.197814
C 4.785398 1.252852 -0.840705	C 4.715550 1.232471 -1.005392
H 4.829627 2.012862 -1.647300	H 4.639004 1.915531 -1.875006
H 5.378261 1.618528 0.021685	H 5.237403 1.767403 -0.187102
H 5.245939 0.313105 -1.208864	H 5.307602 0.341817 -1.291220
C 2.427988 0.436533 -1.483961	C 2.488336 0.023215 -1.536928
H 1.441950 0.158003 -1.065807	H 1.550818 -0.342667 -1.074406
H 2.881410 -0.421776 -2.014031	H 3.057956 -0.804820 -1.995845
I 1.951091 1.916835 -3.094216	I 1.782797 1.290014 -3.227046
C 3.681471 -2.028007 0.417360	C 4.005842 -1.321360 0.731956
O 4.199744 -2.165183 -0.635492	O 4.578439 -1.779104 -0.237081
O 3.215269 -2.322496 1.483058	O 3.755562 -1.749274 1.911212
I_{CD} (X = I)	**D** (X = I)
SCF Done: -4501.93121864 A.U.	SCF Done: -4501.94407121 A.U.
Si -2.411365 1.589538 -2.227766	Si -2.372316 1.214913 -2.175591
Si -5.008467 -0.806070 -0.121346	Si -4.829635 -1.042099 0.094531
Si -2.686612 -2.412425 1.023741	Si -2.373695 -2.384875 1.359823
Si -0.709937 3.291432 -0.103404	Si -0.802747 3.346020 -0.359545
Si -4.516900 1.996067 1.189098	Si -4.516048 1.904495 1.165814
Si -0.976762 -0.895331 -0.948264	Si -0.725443 -1.150514 -0.813179
Si -1.794313 2.404959 2.707797	Si -1.778317 2.698126 2.441385
O -1.208217 3.372660 1.496053	O -1.416821 3.710677 1.183987
O -4.274346 0.655072 0.218040	O -4.224055 0.494155 0.320706
O -1.959397 0.004734 -1.923919	O -1.852907 -0.299149 -1.661225
O -3.400004 2.054425 2.416063	O -3.352420 2.156984 2.327114
O -4.289578 -2.035554 0.753225	O -3.989056 -2.147182 1.022116
O -1.830304 -2.232149 -0.404765	O -1.493686 -2.439426 -0.066341
O -1.945136 2.587175 -0.977022	O -1.972182 2.354784 -1.029858
O -2.048206 -1.368186 2.147357	O -1.813396 -1.077232 2.233696
O -0.520498 -0.008573 0.392363	O -0.017867 -0.226749 0.397219
O -0.931566 0.999603 2.849349	O -0.738303 1.404374 2.456322
H -3.903973 1.631732 -2.303026	H -3.864909 1.161903 -2.247225

H -4.868078 -1.056283 -1.586754	H -4.708762 -1.380719 -1.354918
H 0.202200 -1.383431 -1.704327	H 0.335933 -1.670350 -1.706197
H -6.446860 -0.760507 0.301325	H -6.257155 -1.093164 0.554862
H -4.433427 3.215280 0.330898	H -4.558250 3.037684 0.194274
H -1.799603 2.029947 -3.514793	H -1.773249 1.510773 -3.505780
H -0.547016 4.705704 -0.561062	H -0.713899 4.651441 -1.065592
H -5.865598 1.868251 1.834989	H -5.821076 1.754381 1.892983
H 0.562889 2.528364 -0.182450	H 0.488031 2.647279 -0.118114
H -2.633261 -3.822814 1.476573	H -2.258717 -3.659893 2.097379
H -1.703996 3.139723 3.991602	H -1.641493 3.427789 3.726286
Si -0.669623 -0.415492 2.026992	Si -0.428251 -0.157270 2.035234
O 0.632502 -1.195597 2.580646	O 0.796773 -0.757418 2.930179
Y 2.685386 -1.503942 2.798200	Y 2.084342 -2.368087 3.033790
Cl 3.823926 0.596047 3.589967	Cl 3.813508 -2.272832 4.852981
Cl 2.994742 -3.394211 4.425456	Cl 0.713032 -4.452250 2.839832
O 2.699571 -0.558874 0.423963	O 3.105422 0.124479 0.624625
C 2.633222 0.557849 -0.538557	C 2.887780 1.022592 -0.543005
H 1.570634 0.854551 -0.508433	H 1.826163 1.335247 -0.476747
C 3.542481 1.675878 -0.062363	C 3.819595 2.206555 -0.466075
H 3.389531 2.561159 -0.709772	H 3.610206 2.851159 -1.345286
H 3.306690 1.933448 0.988377	H 3.624084 2.794903 0.451906
H 4.607134 1.367626 -0.113773	H 4.882480 1.887787 -0.480811
C 3.002349 -0.046530 -1.886432	C 3.098736 0.054624 -1.722401
H 2.290499 -0.706892 -2.395505	H 2.309698 0.150879 -2.492503
H 3.830603 0.359562 -2.475830	H 4.099823 0.139385 -2.192822
I 1.531456 1.953182 -3.369719	I 1.192835 2.725996 -3.378690
C 3.575895 -1.541189 0.035645	C 3.045262 -1.127396 0.215055
O 4.019162 -1.453195 -1.148348	O 3.017166 -1.272087 -1.099095
O 3.808737 -2.397737 0.930022	O 3.029596 -2.100521 0.994085
Model B2:	
Y (X = Br)	**Y-PO** (X = Br)
SCF Done: -3855.11996201 A.U.	SCF Done: -4048.14550340 A.U.
Si -4.300529 2.143388 -1.059731	Si 3.724446 -0.514239 -0.512912
Si -2.645707 -1.239562 0.851927	Si 0.538878 2.303361 -0.669036
Si -1.355823 -1.737711 -1.844424	Si -0.005711 -0.454692 -2.085217
Si -2.981344 2.547410 1.818633	Si 4.525821 -1.518728 2.378454
Si -0.101147 -0.911105 2.665625	Si 0.666888 1.406095 2.359779
Si -2.300301 0.838789 -3.241712	Si 2.132068 -2.581670 -2.186274
Si 0.043545 1.810566 1.156283	Si 1.484049 -1.587143 2.731315
O -1.341318 2.257211 1.938320	O 3.046917 -1.169929 3.097306
O -1.654661 -1.307444 2.180929	O 0.080283 1.740754 0.830251
O -3.297918 1.789243 -2.341885	O 3.421384 -1.919243 -1.379827
O 0.504667 0.286278 1.650130	O 0.523264 -0.228845 2.671255
O -2.019191 -2.183318 -0.396421	O 0.436477 1.114215 -1.836827
O -2.386227 -0.745887 -2.689406	O 1.217837 -1.312945 -2.812068
O -3.432794 2.743963 0.227951	O 4.607073 -0.846981 0.852395
O 0.047117 -0.805650 -1.540007	O -0.294948 -1.195906 -0.589838
O -0.705906 1.317765 -3.063531	O 1.127886 -3.421553 -1.133254
O -0.283013 1.729028 -0.475056	O 1.538830 -2.256975 1.199857
H -5.027119 0.898948 -0.641997	H 2.425957 0.121789 -0.120485
H -2.703530 0.162181 0.334132	H 1.953261 2.790474 -0.618144
H -2.678332 0.912111 -4.668388	H 2.594980 -3.481560 -3.261098
H -3.978887 -1.776225 1.236704	H -0.406651 3.392145 -1.065832
H -0.187707 -0.419011 4.070109	H 2.106640 1.813428 2.438131
H -5.232146 3.212768 -1.523224	H 4.545964 0.396376 -1.361406
H -3.717419 1.389154 2.423273	H 5.576197 -0.869833 3.214115
H 0.787234 -2.096110 2.498817	H -0.200629 2.126659 3.335680
H -3.261470 3.820266 2.545496	H 4.701010 -3.001275 2.280317
H -0.962751 -2.945427 -2.599138	H -1.229884 -0.508845 -2.919247
H 1.131845 2.774691 1.436458	H 0.921899 -2.521289 3.731123
Si 0.288974 0.928107 -1.798146	Si 0.340490 -2.663667 0.120306
O 1.887448 0.906912 -2.029656	O -1.019626 -3.210155 0.784772
Y 2.353624 -1.197159 -1.789841	Y -2.410986 -1.520140 0.519098
Cl 2.406822 -2.740316 -3.760824	Cl -4.436362 -2.099823 -0.878705
O 3.242459 -1.753131 -0.051284	O -2.517790 0.643794 -0.484529
C 3.657532 -1.888431 1.285036	C -3.407471 1.232765 -1.475416
H 2.901166 -2.495951 1.838459	C -3.630503 1.501203 -0.039594
C 5.016988 -2.580942 1.374369	H -4.047377 0.493905 -1.989724
H 5.338489 -2.690145 2.429892	H -2.909166 1.996186 -2.098267
H 4.962192 -3.588214 0.915666	H -4.431882 0.910747 0.444004
H 5.783628 -1.990535 0.829345	C -3.228004 2.766277 0.660223

C 3.649836 -0.473216 1.876183 H 2.711982 0.047895 1.615580 H 4.533939 0.120231 1.571184 Br 3.657817 -0.482313 3.904923	H -4.106918 3.437066 0.753553 H -2.863881 2.528580 1.679678 H -2.425740 3.296131 0.112371 O -2.834927 -0.702320 2.345808 C -2.630066 -0.373800 3.693584 H -1.820191 0.391071 3.772754 C -3.908281 0.181432 4.323122 H -3.751982 0.439527 5.390074 H -4.229083 1.095785 3.784067 H -4.725673 -0.566432 4.251079 C -2.122229 -1.652042 4.368283 H -1.296837 -2.097667 3.785124 H -2.926287 -2.398088 4.522047 Br -1.323352 -1.303963 6.198532
$\mathbf{I}_{AB}$ (X = Br)	**B** (X = Br)
SCF Done: -4061.68968774 A.U. Si 3.744099 -0.285645 0.225382 Si 0.559088 2.553019 -0.380535 Si -0.106859 -0.210314 -1.924311 Si 3.785836 -1.922869 2.906554 Si -0.582590 1.549136 2.472093 Si 2.181761 -2.203589 -1.704599 Si 0.856951 -1.141735 3.142473 O 2.440192 -1.280472 3.657474 O 0.360490 1.978085 1.152496 O 3.444829 -1.492659 -0.903400 O 0.354152 0.411811 3.320740 O 0.264928 1.329663 -1.501294 O 1.260737 -1.014054 -2.443812 O 4.305322 -0.962417 1.640844 O -0.739351 -1.084182 -0.618046 O 1.169720 -3.027458 -0.663421 O 0.896584 -1.564397 1.519586 H 2.511735 0.513056 0.482596 H 1.998175 2.937547 -0.546040 H 2.725817 -3.135341 -2.718415 H -0.365615 3.676461 -0.704385 H -0.736213 2.671290 3.428276 H 4.859446 0.548392 -0.317719 H 4.888229 -1.937126 3.915477 H -1.792412 0.806349 2.026240 H 3.491273 -3.301127 2.393726 H -1.110861 -0.203943 -3.014242 H 0.008853 -2.078382 3.918958 Si 0.028333 -2.321611 0.331891 O -1.249424 -3.182482 0.778390 Y -3.004870 -1.945563 0.246457 Cl -4.737884 -3.566206 -0.632867 O -3.664655 0.012569 -0.745716 C -3.988490 1.298974 0.313543 C -2.974326 1.293256 -0.725705 H -3.761769 0.928794 1.321264 H -4.993821 1.683547 0.091841 H -1.939274 1.206838 -0.347704 C -3.115709 2.146460 -1.958730 H -2.818647 3.181668 -1.695135 H -2.464463 1.781194 -2.777342 H -4.167053 2.151641 -2.309582 Br -2.980683 3.705239 1.449953 O -3.351132 -1.269378 2.163257 C -3.170010 -1.369030 3.549282 H -2.269438 -0.779552 3.856402 C -4.388831 -0.826339 4.295924 H -4.254322 -0.894689 5.394475 H -4.545945 0.236861 4.024414 H -5.295572 -1.398940 4.006513 C -2.880154 -2.851024 3.807087 H -2.028638 -3.200467 3.192847 H -3.772230 -3.481630 3.623272 Br -2.335104 -3.243676 5.735853	SCF Done: -4061.72450255 A.U. Si -2.388573 1.888734 -0.907859 Si -3.310253 -1.256595 1.943259 Si -0.974670 -2.641832 0.330071 Si 0.297696 3.547508 -0.495621 Si -2.485216 1.521374 3.435019 Si -0.923327 -0.688744 -2.000362 Si 0.357973 1.907644 2.067183 O 0.481772 3.298084 1.152717 O -2.761399 -0.027760 2.910692 O -1.982826 0.583594 -1.867929 O -0.959055 2.052608 3.065528 O -2.076680 -2.285556 1.518598 O -1.511081 -1.988185 -1.119899 O -1.243008 3.089168 -0.975116 O 0.514179 -1.981829 0.668983 O 0.581302 -0.287138 -1.411184 O 0.092282 0.634297 1.027936 H -2.597010 1.447813 0.503661 H -3.947255 -0.689527 0.709245 H -0.834003 -1.055407 -3.434348 H -4.291988 -2.054465 2.742572 H -3.494389 2.441465 2.810812 H -3.648781 2.452819 -1.483265 H 0.398255 5.013047 -0.746482 H -2.612966 1.526039 4.926036 H 1.298821 2.743230 -1.258847 H -0.865541 -4.114637 0.222493 H 1.572171 1.762099 2.900856 Si 1.064132 -0.457608 0.192437 O 2.633031 -0.247007 0.439163 Y 3.963750 -0.417456 2.130794 Cl 5.625784 -2.329367 1.814083 O 2.655776 -0.818661 3.712872 C 1.695646 -1.632590 4.318780 H 1.951506 -1.798735 5.396934 C 0.299357 -1.009436 4.229746 H -0.462651 -1.620314 4.753731 H 0.315933 0.002181 4.682362 H -0.007080 -0.918153 3.169288 C 1.808008 -2.968642 3.575424 H 2.816528 -3.409418 3.679088 H 1.528118 -2.851323 2.510970 Br 0.537909 -4.430827 4.268215 O 4.848834 1.489023 2.293380 C 5.158506 2.631892 1.554556 H 5.543538 3.442393 2.226075 C 6.210464 2.346075 0.475800 H 6.481509 3.259374 -0.092901 H 7.123962 1.935671 0.951944 H 5.825672 1.587561 -0.240416 C 3.809041 3.078990 0.985062 H 3.084303 3.297051 1.787501 H 3.397106 2.324510 0.285560 Br 3.858281 4.824369 -0.102054
$\mathbf{I}_{BC}$ (X = Br)	**C** (X = Br)

SCF Done: -4250.19079361 A.U.			
Si	-2.671019	1.696746	-1.877176
Si	-5.523476	-0.960988	0.031295
Si	-2.983605	-2.734958	0.493828
Si	-0.626241	3.021174	0.080697
Si	-5.556579	1.929468	1.491103
Si	-1.315359	-1.156770	-1.482564
Si	-2.487060	1.977057	2.211129
O	-1.752129	3.171036	1.321432
O	-5.683391	0.325088	1.068499
O	-2.122144	0.137054	-2.126420
O	-4.126908	2.266094	2.261793
O	-4.525529	-2.133111	0.670785
O	-2.422192	-2.337037	-1.035422
O	-1.486502	2.722800	-1.337559
O	-1.949267	-2.106024	1.633207
O	-0.464910	-0.726199	-0.114558
O	-2.264059	0.529015	1.410768
H	-3.805861	1.660433	-0.902238
H	-5.001936	-0.507918	-1.296625
H	-0.394775	-1.706890	-2.505214
H	-6.880675	-1.582163	-0.101080
H	-5.705968	2.783082	0.266320
H	-3.131153	2.196149	-3.209602
H	0.067177	4.324600	-0.094847
H	-6.654382	2.212017	2.469738
H	0.277283	1.862589	0.309055
H	-3.053228	-4.209144	0.645418
H	-1.997572	1.949592	3.608825
Si	-1.088069	-0.668944	1.458786
O	0.044772	-0.420138	2.563685
Y	1.937854	0.558062	2.864477
Cl	1.356340	3.055398	2.887805
O	3.111583	0.582294	1.046999
C	3.155286	1.396176	-0.103882
H	2.621297	2.356143	0.105044
C	4.596117	1.711106	-0.509374
H	4.624944	2.346271	-1.418725
H	5.104157	2.251252	0.314899
H	5.152383	0.772075	-0.709156
C	2.361026	0.636854	-1.171867
H	1.390759	0.296645	-0.765945
H	2.926745	-0.211670	-1.599717
Br	1.860283	1.806489	-2.764638
C	3.607341	-1.545225	1.060754
O	4.242284	-1.720703	0.081605
O	3.036706	-1.747623	2.091547
O	2.934926	0.187774	4.661317
C	4.028620	0.047409	5.506793
H	3.760849	-0.579094	6.397065
C	5.221926	-0.598739	4.791767
H	6.093867	-0.720839	5.466679
H	4.924971	-1.594171	4.404710
H	5.527337	0.028453	3.925812
C	4.313500	1.472100	5.996595
H	3.417563	1.917630	6.464623
H	4.684946	2.121013	5.179676
Br	5.760679	1.574204	7.454699

SCF Done: -4250.20381398 A.U.			
Si	-2.725114	1.896301	-1.669792
Si	-5.515408	-0.629587	0.445813
Si	-3.143047	-2.672158	0.354275
Si	-0.322096	2.845695	0.045286
Si	-4.970003	2.086983	2.168311
Si	-1.595046	-1.079611	-1.716631
Si	-1.857523	1.766328	2.397936
O	-1.242084	2.981701	1.446300
O	-5.355605	0.589870	1.556769
O	-2.324638	0.344284	-2.142972
O	-3.433104	2.128851	2.796298
O	-4.557761	-1.937725	0.834307
O	-2.768966	-2.163459	-1.198358
O	-1.397554	2.802298	-1.253818
O	-1.883779	-2.282898	1.367778
O	-0.521838	-0.871892	-0.455833
O	-1.882484	0.376587	1.477656
H	-3.681798	1.825421	-0.521380
H	-5.172002	-0.138906	-0.926246
H	-0.898295	-1.634984	-2.899348
H	-6.936131	-1.099620	0.517204
H	-5.125561	3.118613	1.090385
H	-3.361349	2.547324	-2.856289
H	0.494694	4.078706	-0.119816
H	-5.908047	2.356123	3.303358
H	0.454788	1.579944	0.019937
H	-3.363168	-4.138983	0.375861
H	-1.107592	1.606247	3.664640
Si	-0.887519	-0.939103	1.193020
O	0.428923	-0.970431	2.108950
Y	2.281125	-0.142794	2.742657
Cl	1.968613	2.413667	2.509862
O	3.425626	0.127604	0.639436
C	3.271810	0.856711	-0.603863
H	2.669826	1.734093	-0.289080
C	4.614808	1.312198	-1.160456
H	4.452972	1.931199	-2.065933
H	5.143752	1.927638	-0.405778
H	5.241303	0.437447	-1.420234
C	2.430591	-0.013474	-1.535457
H	1.548250	-0.426990	-1.011161
H	3.020632	-0.808964	-2.024129
Br	1.622530	1.092515	-3.031788
C	4.079584	-1.190450	0.723753
O	4.648387	-1.656959	-0.244728
O	3.873273	-1.598803	1.919627
O	2.464801	-0.280667	4.806120
C	2.447011	0.292221	6.078064
H	2.369816	-0.504448	6.861746
C	3.711100	1.121020	6.333715
H	3.717183	1.562764	7.351184
H	4.604297	0.472999	6.221348
H	3.778454	1.941714	5.587737
C	1.159102	1.124941	6.104936
H	0.275964	0.495955	5.889802
H	1.211803	1.977204	5.399329
Br	0.751261	1.957941	7.936042

$\mathbf{I}_{CD}$ (X = Br)			
SCF Done: -4250.18054903 A.U.			
Si	-2.360664	1.586270	-2.118493
Si	-5.115262	-0.606669	-0.189014
Si	-2.866625	-2.598216	0.539042
Si	-0.660934	3.374922	-0.036845
Si	-4.323050	1.945250	1.490237
Si	-1.103276	-1.303847	-1.477168
Si	-1.385436	1.979327	2.524620
O	-1.011957	3.318257	1.602967
O	-4.318456	0.772233	0.301307
O	-2.111185	-0.037384	-1.828735
O	-3.043806	1.763888	2.536739

D (X = Br)			
SCF Done: -4250.18954501 A.U.			
Si	-0.197398	1.157017	-1.118209
Si	-4.342321	0.562125	0.049745
Si	-3.971090	-2.483426	-0.409354
Si	1.250861	0.451579	1.706627
Si	-2.315239	1.997191	1.966374
Si	-1.375358	-1.666506	-1.624674
Si	-1.080030	-0.566328	3.230743
O	0.534562	-0.754217	2.689090
O	-2.887745	1.124503	0.660484
O	-1.163435	-0.026119	-1.789645
O	-1.496916	1.033133	3.061894

O -4.411009 -1.979345 0.448441	O -4.555847 -1.077850 0.278403
O -2.123243 -2.542422 -0.955734	O -3.007716 -2.036162 -1.710006
O -1.842114 2.515991 -0.835796	O 0.196094 0.806271 0.467569
O -1.971205 -1.689042 1.606869	O -3.047659 -3.341696 0.683035
O -0.085681 -0.966120 -0.192818	O -0.826302 -2.108206 -0.123165
O -0.662759 0.682414 1.807898	O -2.037174 -1.479677 2.249213
H -3.840775 1.772001 -2.222335	H -0.960384 2.439637 -1.148554
H -5.089449 -0.648862 -1.681480	H -4.350823 0.876985 -1.410820
H -0.336435 -1.793685 -2.641675	H -0.664087 -2.374416 -2.715682
H -6.521587 -0.577478 0.334989	H -5.458376 1.239762 0.785633
H -4.274048 3.280048 0.818322	H -1.377162 3.046158 1.471051
H -1.691483 2.010231 -3.383379	H 1.075529 1.248048 -1.902361
H -0.745155 4.816473 -0.435147	H 1.400957 1.683859 2.537216
H -5.573405 1.791336 2.306519	H -3.482693 2.603755 2.688184
H 0.693190 2.814663 -0.296068	H 2.546524 -0.058952 1.196624
H -2.993783 -4.006166 0.990055	H -5.102151 -3.323708 -0.866670
H -0.949687 2.182443 3.923204	H -1.155775 -0.934252 4.658706
Si -0.487522 -0.925102 1.443500	Si -1.576167 -2.749892 1.240694
O 0.649614 -1.599091 2.377530	O -0.558123 -3.737297 1.998850
Y 2.469759 -0.917945 3.204289	Y 1.434457 -3.298387 2.670431
Cl 2.383364 1.525942 3.910290	Cl 2.513562 -5.489466 3.299427
O 2.914869 -0.071557 0.869530	O 2.888875 -2.001879 4.443412
C 2.609873 0.701631 -0.346489	C 3.936571 -1.068014 4.985277
H 1.525685 0.893072 -0.280437	H 4.904696 -1.588675 4.886252
C 3.424837 1.981371 -0.320889	C 3.893349 0.219961 4.193664
H 3.140119 2.605205 -1.190281	H 4.704689 0.866776 4.588075
H 3.214853 2.536448 0.614097	H 4.074769 0.022800 3.118819
H 4.511008 1.758804 -0.373040	H 2.917376 0.733966 4.319266
C 2.895965 -0.235696 -1.511102	C 3.497775 -0.964870 6.460161
H 2.190539 -1.049522 -1.711800	H 4.069956 -1.621539 7.138986
H 3.606482 0.037222 -2.297544	H 3.490991 0.063601 6.855854
Br 1.223879 1.116147 -3.074365	Br 6.441661 0.170125 6.701510
C 3.766352 -1.122356 0.641232	C 1.857422 -2.075963 5.309340
O 4.099634 -1.308962 -0.568568	O 2.080020 -1.451040 6.442204
O 4.072001 -1.769641 1.677997	O 0.832855 -2.682992 4.982356
O 2.832543 -1.892060 4.992275	O 2.512242 -2.607036 1.061531
C 3.052284 -1.940998 6.369667	C 3.254628 -2.364622 -0.091483
H 2.928381 -2.988510 6.745523	H 3.853334 -1.423269 0.024029
C 4.459164 -1.446622 6.724311	C 4.206418 -3.522028 -0.399749
H 4.652978 -1.499006 7.815093	H 4.803005 -3.326412 -1.313865
H 5.211892 -2.068915 6.198717	H 4.896956 -3.671121 0.454018
H 4.581418 -0.393853 6.390642	H 3.627821 -4.459647 -0.538111
C 1.935618 -1.076287 6.967407	C 2.203962 -2.119726 -1.178384
H 0.939778 -1.454402 6.672225	H 1.508495 -1.324541 -0.861175
H 2.048946 -0.012849 6.678583	H 1.637970 -3.039477 -1.417178
Br 1.893650 -1.088064 9.016250	Br 2.966918 -1.463421 -2.948656
$\mathbf{I}_{AB}$ (X = I)	**B** (X = I)
SCF Done: -4059.75284748 A.U.	SCF Done: -4059.75284748 A.U.
Si 3.733046 -0.293435 0.221001	Si 3.733046 -0.293435 0.221001
Si 0.592397 2.508794 -0.448015	Si 0.592397 2.508794 -0.448015
Si -0.112873 -0.261266 -1.940816	Si -0.112873 -0.261266 -1.940816
Si 3.811514 -1.922188 2.908331	Si 3.811514 -1.922188 2.908331
Si -0.550748 1.549171 2.457108	Si -0.550748 1.549171 2.457108
Si 2.196809 -2.229484 -1.710465	Si 2.196809 -2.229484 -1.710465
Si 0.881748 -1.150410 3.144224	Si 0.881748 -1.150410 3.144224
O 2.462451 -1.286819 3.662146	O 2.462451 -1.286819 3.662146
O 0.313352 1.982976 1.088409	O 0.313352 1.982976 1.088409
O 3.451773 -1.497844 -0.914168	O 3.451773 -1.497844 -0.914168
O 0.397635 0.417221 3.279293	O 0.397635 0.417221 3.279293
O 0.241020 1.294379 -1.555239	O 0.241020 1.294379 -1.555239
O 1.261655 -1.055368 -2.457072	O 1.261655 -1.055368 -2.457072
O 4.310476 -0.965114 1.631802	O 4.310476 -0.965114 1.631802
O -0.711214 -1.110098 -0.604339	O -0.711214 -1.110098 -0.604339
O 1.196324 -3.055038 -0.659328	O 1.196324 -3.055038 -0.659328
O 0.917073 -1.607587 1.533234	O 0.917073 -1.607587 1.533234
H 2.483855 0.476653 0.487720	H 2.483855 0.476653 0.487720
H 2.051183 2.820687 -0.586068	H 2.051183 2.820687 -0.586068
H 2.750056 -3.162642 -2.717416	H 2.750056 -3.162642 -2.717416
H -0.260972 3.679322 -0.806890	H -0.260972 3.679322 -0.806890
H -0.676466 2.708083 3.374574	H -0.676466 2.708083 3.374574
H 4.826590 0.568940 -0.320576	H 4.826590 0.568940 -0.320576

H 4.918859 -1.915778 3.911228	H 4.918859 -1.915778 3.911228
H -1.803176 0.855357 2.050370	H -1.803176 0.855357 2.050370
H 3.526281 -3.306647 2.408225	H 3.526281 -3.306647 2.408225
H -1.131613 -0.285344 -3.015885	H -1.131613 -0.285344 -3.015885
H 0.020803 -2.050388 3.947716	H 0.020803 -2.050388 3.947716
Si 0.052488 -2.357116 0.337305	Si 0.052488 -2.357116 0.337305
O -1.228855 -3.216653 0.774326	O -1.228855 -3.216653 0.774326
Y -2.967094 -1.952462 0.238571	Y -2.967094 -1.952462 0.238571
Cl -4.728838 -3.535394 -0.649503	Cl -4.728838 -3.535394 -0.649503
O -3.561625 0.012538 -0.770266	O -3.561625 0.012538 -0.770266
C -4.106813 1.219709 0.270789	C -4.106813 1.219709 0.270789
C -2.984051 1.344045 -0.646592	C -2.984051 1.344045 -0.646592
H -3.952363 0.851557 1.294023	H -3.952363 0.851557 1.294023
H -5.111655 1.526589 -0.050768	H -5.111655 1.526589 -0.050768
H -1.991577 1.326022 -0.159294	H -1.991577 1.326022 -0.159294
C -3.065024 2.217530 -1.870720	C -3.065024 2.217530 -1.870720
H -2.902960 3.267991 -1.553617	H -2.902960 3.267991 -1.553617
H -2.288305 1.943416 -2.611302	H -2.288305 1.943416 -2.611302
H -4.064593 2.135211 -2.342309	H -4.064593 2.135211 -2.342309
I -3.516452 3.899245 1.671605	I -3.516452 3.899245 1.671605
O -3.297366 -1.251184 2.149156	O -3.297366 -1.251184 2.149156
C -3.150631 -1.352942 3.539714	C -3.150631 -1.352942 3.539714
H -2.265123 -0.752982 3.870121	H -2.265123 -0.752982 3.870121
C -4.393937 -0.828758 4.258010	C -4.393937 -0.828758 4.258010
H -4.284469 -0.899456 5.359177	H -4.284469 -0.899456 5.359177
H -4.560084 0.233111 3.987210	H -4.560084 0.233111 3.987210
H -5.285082 -1.413665 3.945610	H -5.285082 -1.413665 3.945610
C -2.849198 -2.832136 3.801575	C -2.849198 -2.832136 3.801575
H -1.988109 -3.175264 3.197310	H -1.988109 -3.175264 3.197310
H -3.732767 -3.471683 3.607508	H -3.732767 -3.471683 3.607508
Br -2.323146 -3.217844 5.735840	Br -2.323146 -3.217844 5.735840
I_{BC} (X = I)	**C** (X = I)
SCF Done: -4248.25319190 A.U.	SCF Done: -4248.26505817 A.U.
Si -2.148368 1.490705 -1.836284	Si -2.760989 1.952059 -1.642158
Si -5.164212 -1.375614 -0.261889	Si -5.498259 -0.664904 0.592758
Si -2.607593 -2.770886 0.844629	Si -3.132863 -2.687429 0.329140
Si -0.752847 3.159749 0.485983	Si -0.280976 2.837829 0.029775
Si -5.784483 1.609230 0.741379	Si -4.959205 2.012957 2.299364
Si -0.697266 -1.179063 -0.909772	Si -1.712347 -1.036109 -1.790025
Si -2.984371 2.000140 2.159115	Si -1.828066 1.742665 2.366039
O -2.062313 3.233804 1.534518	O -1.189937 2.964494 1.438566
O -5.697134 -0.045801 0.582942	O -5.332338 0.471053 1.793962
O -1.369924 0.009588 -1.848973	O -2.478048 0.386817 -2.157701
O -4.566923 2.214074 1.691641	O -3.382571 2.140417 2.804482
O -4.213156 -2.354164 0.696291	O -4.542271 -1.999075 0.887402
O -1.827072 -2.378559 -0.587593	O -2.846045 -2.141236 -1.229256
O -1.295381 2.657702 -1.024264	O -1.364063 2.762323 -1.259643
O -1.879977 -1.962946 2.105000	O -1.835219 -2.282256 1.287333
O -0.212687 -0.552525 0.554457	O -0.583362 -0.823085 -0.579798
O -2.459593 0.559682 1.496598	O -1.908797 0.377413 1.408707
H -3.502942 1.330041 -1.221111	H -3.683640 1.921725 -0.464530
H -4.409285 -0.954637 -1.483950	H -5.157952 -0.075004 -0.740281
H 0.446699 -1.764579 -1.645150	H -1.076540 -1.571718 -3.015040
H -6.379783 -2.175917 -0.617394	H -6.918626 -1.139198 0.635632
H -5.745280 2.248096 -0.615415	H -5.231951 2.981817 1.186453
H -2.257863 1.918822 -3.263731	H -3.393751 2.661490 -2.797096
H -0.197965 4.528045 0.327362	H 0.511304 4.085048 -0.148249
H -7.076521 1.915227 1.433600	H -5.819471 2.308028 3.487572
H 0.227211 2.132486 0.930061	H 0.529237 1.591246 0.007195
H -2.537458 -4.232258 1.089922	H -3.315504 -4.159373 0.335457
H -2.937595 2.013845 3.640508	H -1.054988 1.526418 3.610957
Si -1.177834 -0.442332 1.939479	Si -0.885157 -0.910181 1.080247
O -0.346459 0.114205 3.192252	O 0.461592 -0.901389 1.949983
Y 1.610892 1.058785 3.169661	Y 2.273118 -0.095169 2.714407
Cl 1.235603 3.598153 3.263957	Cl 2.041881 2.468661 2.488673
O 2.651234 0.934736 1.257691	O 3.490453 0.142081 0.647279
C 3.007823 1.788788 0.189816	C 3.355198 0.837813 -0.619240
H 2.668548 2.824127 0.439282	H 2.764908 1.732181 -0.330110
C 4.525185 1.795381 -0.008595	C 4.712605 1.258121 -1.170791
H 4.829905 2.476936 -0.828480	H 4.578833 1.870519 -2.085025
H 5.014021 2.134498 0.926939	H 5.245044 1.870228 -0.415829

H	4.885459	0.772243	-0.241658	H	5.324517	0.367878	-1.411108
C	2.207006	1.302361	-1.026743	C	2.509074	-0.060845	-1.520145
H	1.132116	1.242906	-0.784346	H	1.593244	-0.404736	-1.001625
H	2.570625	0.333501	-1.412732	H	3.088467	-0.913279	-1.918982
I	2.293683	2.694117	-2.773681	I	1.712081	1.025569	-3.289819
C	2.754042	-1.127944	1.187065	C	4.147731	-1.170095	0.783842
O	3.194073	-1.428326	0.129256	O	4.748912	-1.659133	-0.153251
O	2.325242	-1.302788	2.295828	O	3.906425	-1.549720	1.983114
O	2.911096	0.652026	4.749860	O	2.329446	-0.255763	4.784093
C	4.175159	0.287919	5.206759	C	2.324754	0.318391	6.055699
H	4.359019	0.714294	6.226680	H	2.211602	-0.473703	6.839597
C	4.336615	-1.235218	5.269780	C	3.617489	1.099619	6.319205
H	5.336161	-1.528099	5.651549	H	3.634291	1.541230	7.336601
H	3.559823	-1.658712	5.938171	H	4.486697	0.418919	6.211808
H	4.191048	-1.671879	4.259664	H	3.718861	1.917348	5.573722
C	5.142683	0.962946	4.226640	C	1.070223	1.200562	6.071844
H	4.981002	2.056092	4.197446	H	0.164311	0.606539	5.852774
H	5.061725	0.530798	3.209707	H	1.162200	2.047915	5.364415
Br	7.128112	0.759189	4.722895	Br	0.683209	2.054232	7.897958
I_{CD} (X = I)				**D** (X = I)			
SCF Done: -4248.24060442 A.U.				SCF Done: -4248.25489317 A.U.			
Si	-2.464341	1.581193	-2.105397	Si	-0.193068	1.151204	-1.125951
Si	-5.149504	-0.619255	-0.106123	Si	-4.338041	0.574128	0.048543
Si	-2.878734	-2.593533	0.573880	Si	-3.981967	-2.472772	-0.415288
Si	-0.678471	3.315099	-0.083112	Si	1.256751	0.438939	1.698929
Si	-4.320515	1.943515	1.530508	Si	-2.302185	1.998008	1.964699
Si	-1.148980	-1.297631	-1.473227	Si	-1.383785	-1.667239	-1.634598
Si	-1.362050	2.010788	2.526188	Si	-1.075569	-0.573242	3.223610
O	-0.988008	3.323149	1.565557	O	0.539349	-0.766094	2.682553
O	-4.320263	0.749328	0.360535	O	-2.880211	1.128987	0.659038
O	-2.154943	-0.036302	-1.846698	O	-1.163518	-0.027852	-1.797810
O	-3.020188	1.799907	2.556018	O	-1.485725	1.027500	3.056503
O	-4.433847	-2.000238	0.500594	O	-4.557254	-1.065283	0.276085
O	-2.156353	-2.534535	-0.931991	O	-3.017957	-2.028858	-1.716553
O	-1.938668	2.510601	-0.823502	O	0.206945	0.790245	0.456297
O	-1.983194	-1.657899	1.617041	O	-3.060398	-3.336914	0.674661
O	-0.124269	-0.919386	-0.206422	O	-0.833775	-2.113422	-0.134328
O	-0.648430	0.693708	1.839643	O	-2.035377	-1.483461	2.242337
H	-3.948655	1.733797	-2.183485	H	-0.953797	2.435187	-1.145833
H	-5.171648	-0.657937	-1.599069	H	-4.345854	0.890376	-1.411632
H	-0.378194	-1.788734	-2.634903	H	-0.677901	-2.377694	-2.727334
H	-6.537248	-0.578750	0.463767	H	-5.450186	1.255660	0.786470
H	-4.307178	3.268678	0.838938	H	-1.358447	3.041700	1.469104
H	-1.815587	2.031840	-3.372762	H	1.076753	1.243576	-1.914609
H	-0.677366	4.747065	-0.519147	H	1.403649	1.671935	2.529417
H	-5.553065	1.780062	2.371505	H	-3.464653	2.609155	2.690159
H	0.620923	2.649310	-0.374822	H	2.556074	-0.070872	1.197193
H	-2.976199	-4.000505	1.034352	H	-5.117791	-3.307008	-0.871371
H	-0.913086	2.249571	3.914607	H	-1.151466	-0.943113	4.651162
Si	-0.494702	-0.906187	1.439241	Si	-1.585109	-2.753411	1.228916
O	0.649178	-1.609287	2.341728	O	-0.569561	-3.747642	1.983029
Y	2.465712	-0.931825	3.181753	Y	1.423113	-3.315860	2.650508
Cl	2.412367	1.519364	3.866828	Cl	2.502483	-5.504604	3.280275
O	2.912926	-0.114044	0.830774	O	2.913263	-2.008472	4.457407
C	2.671602	0.688784	-0.381334	C	3.933991	-1.058702	5.008788
H	1.579536	0.849442	-0.376770	H	4.911428	-1.567890	4.933000
C	3.444723	1.988974	-0.253827	C	3.886599	0.222004	4.204724
H	3.195070	2.645392	-1.109857	H	4.677343	0.895855	4.594670
H	3.163879	2.494484	0.690713	H	4.085977	0.016492	3.134687
H	4.538213	1.798946	-0.250337	H	2.901204	0.722063	4.310336
C	3.066454	-0.204707	-1.548355	C	3.462766	-0.948429	6.474557
H	2.401296	-1.032106	-1.821779	H	4.025702	-1.597452	7.169689
H	3.826995	0.105248	-2.271435	H	3.451684	0.083527	6.863011
I	1.383149	1.213317	-3.409262	I	6.667080	0.253072	6.958294
C	3.828228	-1.118426	0.644158	C	1.861411	-2.076906	5.298323
O	4.246167	-1.273173	-0.542828	O	2.053946	-1.432637	6.428348
O	4.104718	-1.761843	1.692236	O	0.846563	-2.691724	4.960133
O	2.796098	-1.900504	4.978143	O	2.504442	-2.615259	1.048991
C	3.005099	-1.945605	6.357479	C	3.246724	-2.376463	-0.105557
H	2.863903	-2.989425	6.737297	H	3.849777	-1.437986	0.009840
C	4.416085	-1.468908	6.719764	C	4.192542	-3.538363	-0.414847

H 4.600921 -1.517469 7.812262	H 4.788497 -3.345496 -1.329926
H 5.163951 -2.104667 6.203477	H 4.883991 -3.690831 0.437576
H 4.555495 -0.420005 6.380767	H 3.609424 -4.473265 -0.552512
C 1.896322 -1.062649 6.943251	C 2.196537 -2.126439 -1.191791
H 0.897395 -1.427671 6.642005	H 1.503369 -1.329981 -0.872789
H 2.027021 -0.002070 6.651226	H 1.627824 -3.044092 -1.432239
Br 1.838943 -1.065373 8.991374	Br 2.961719 -1.469467 -2.959884
Model B2 (with I in the ligand):	
Y (X = I)	**Y-PO** (X = I)
SCF Done: -3853.19010032 A.U.	SCF Done: -4046.20767784 A.U.
Si 4.141254 -0.832416 -0.337127	Si 3.730374 -0.508036 -0.503316
Si -0.307485 2.306299 -0.868860	Si 0.538619 2.302571 -0.729496
Si 0.400649 -0.294731 -2.194643	Si 0.002972 -0.477455 -2.094152
Si 4.481996 -1.793474 2.649320	Si 4.522631 -1.489047 2.395372
Si 0.101633 1.603686 2.093577	Si 0.643159 1.491482 2.323290
Si 2.328813 -2.602087 -2.057512	Si 2.134352 -2.611919 -2.132975
Si 1.446180 -1.363847 2.691658	Si 1.482839 -1.503997 2.769505
O 3.012643 -1.168711 3.181743	O 3.055032 -1.107476 3.119941
O -0.733575 1.477526 0.586574	O 0.073625 1.756391 0.773870
O 3.649336 -2.232739 -1.132990	O 3.422524 -1.928206 -1.343471
O 0.770960 0.126423 2.391317	O 0.545664 -0.131731 2.696347
O 0.642686 1.318273 -1.838010	O 0.458982 1.092325 -1.877407
O 1.750398 -1.131295 -2.670096	O 1.221460 -1.361800 -2.797133
O 4.834007 -1.223807 1.121302	O 4.611400 -0.820244 0.867939
O -0.028703 -0.936452 -0.692346	O -0.298819 -1.182598 -0.583994
O 1.098808 -3.297459 -1.135301	O 1.128069 -3.421081 -1.058455
O 1.499510 -2.183014 1.234857	O 1.520301 -2.196635 1.247216
H 2.957928 0.060801 -0.117338	H 2.433732 0.138839 -0.123347
H 0.508825 3.494378 -0.490245	H 1.947601 2.804555 -0.675316
H 2.680099 -3.527798 -3.153018	H 2.598469 -3.541782 -3.181433
H -1.597237 2.621245 -1.540007	H -0.414129 3.375557 -1.151643
H 1.185796 2.608828 1.870642	H 2.067943 1.947907 2.408983
H 5.195132 -0.170725 -1.159550	H 4.555602 0.383508 -1.368238
H 5.528873 -1.281205 3.578507	H 5.590799 -0.860865 3.224236
H -0.861422 2.007244 3.149121	H -0.261366 2.218453 3.260702
H 4.411186 -3.287385 2.624580	H 4.666844 -2.975097 2.298405
H -0.681901 -0.438794 -3.194810	H -1.219159 -0.539886 -2.930948
H 0.650665 -2.066483 3.722144	H 0.912153 -2.409867 3.790125
Si 0.331201 -2.455041 0.077008	Si 0.331746 -2.631019 0.169331
O -1.134749 -2.715951 0.698363	O -1.035329 -3.162446 0.832946
Y -1.998949 -0.662148 0.576444	Y -2.416518 -1.471664 0.526979
Cl -3.606441 -0.067890 -1.261726	Cl -4.487579 -2.066291 -0.796815
O -2.351478 -0.276282 2.563393	O -2.526378 0.666568 -0.527069
C -2.232818 -0.583318 3.932221	C -3.434908 1.244808 -1.506733
H -1.216449 -0.280899 4.289603	C -3.630331 1.531266 -0.070463
C -3.288373 0.164323 4.745965	H -4.086712 0.501618 -1.999404
H -3.191099 -0.045907 5.830116	H -2.948280 2.000111 -2.148382
H -3.177480 1.255669 4.587214	H -4.423309 0.946673 0.434101
H -4.305918 -0.130217 4.413707	C -3.213744 2.802614 0.608914
C -2.335800 -2.112139 4.018108	H -4.091024 3.473613 0.714947
H -1.655305 -2.595401 3.291364	H -2.828748 2.572044 1.622295
H -3.371659 -2.467629 3.849625	H -2.423418 3.328044 0.039850
I -1.731994 -2.942408 5.995756	O -2.770819 -0.620475 2.355338
	C -2.565353 -0.447122 3.734696
	H -1.667347 0.196403 3.892865
	C -3.785598 0.209046 4.381644
	H -3.634510 0.374388 5.467463
	H -3.977950 1.190809 3.903358
	H -4.684389 -0.426871 4.237852
	C -2.244187 -1.845580 4.275968
	H -1.439999 -2.318547 3.681829
	H -3.135379 -2.503722 4.292326
	I -1.455552 -1.848120 6.362310
$\mathbf{I}_{AB}$ (X = I)	**B** (X = I)
SCF Done: -4057.81496776 A.U.	SCF Done: -4057.85097110 A.U.
Si 3.744241 -0.292209 0.214637	Si -2.426676 1.846498 -0.694915
Si 0.588959 2.509148 -0.439968	Si -3.268355 -1.047144 2.464434
Si -0.109225 -0.255766 -1.945199	Si -1.311956 -2.542999 0.366044
Si 3.817041 -1.921141 2.902702	Si 0.310674 3.448833 -0.597347
Si -0.555507 1.544151 2.462195	Si -2.084114 1.793483 3.430086
Si 2.202924 -2.222319 -1.721004	Si -1.153289 -0.656708 -2.018501

Si 0.886620 -1.156415 3.132955	Si 0.716082 1.809539 1.909078
O 2.467733 -1.281228 3.652535	O 0.954621 3.131657 0.918375
O 0.310922 1.974516 1.093830	O -2.463561 0.187297 3.230380
O 3.457892 -1.493248 -0.922667	O -2.019363 0.759798 -1.900606
O 0.386170 0.404534 3.281590	O -0.535555 2.135545 2.952145
O 0.242207 1.298805 -1.553058	O -2.234010 -2.047131 1.645689
O 1.266938 -1.045942 -2.462995	O -1.869729 -1.815780 -1.040798
O 4.319221 -0.968416 1.624240	O -1.330661 3.091319 -0.597996
O -0.707894 -1.110553 -0.612613	O 0.279318 -2.104787 0.569692
O 1.202723 -3.052107 -0.672744	O 0.420893 -0.440328 -1.525038
O 0.929432 -1.602149 1.518786	O 0.254431 0.532029 0.947194
H 2.498869 0.483814 0.482284	H -2.521308 1.132552 0.612230
H 2.046766 2.826294 -0.575622	H -4.277782 -0.474360 1.511060
H 2.756018 -3.151625 -2.731587	H -1.194482 -1.084922 -3.437393
H -0.268280 3.678399 -0.793707	H -3.933637 -1.867321 3.523462
H -0.673457 2.702415 3.381741	H -3.056169 2.637103 2.656121
H 4.841751 0.565992 -0.325688	H -3.741110 2.450714 -1.073893
H 4.922959 -1.913558 3.907119	H 0.424562 4.913712 -0.847256
H -1.812567 0.859072 2.056224	H -2.172117 2.096736 4.893028
H 3.530337 -3.306503 2.405991	H 0.988486 2.612300 -1.633660
H -1.126682 -0.276970 -3.021510	H -1.423591 -4.015722 0.253704
H 0.033255 -2.072801 3.926537	H 1.952240 1.563440 2.681136
Si 0.061254 -2.355479 0.327370	Si 0.998664 -0.672521 0.039844
O -1.217098 -3.216140 0.770604	O 2.597195 -0.684347 0.156000
Y -2.959517 -1.957502 0.238410	Y 4.020552 -0.656644 1.774377
Cl -4.719934 -3.546029 -0.640519	Cl 6.114048 -2.046224 1.294326
O -3.559981 0.006302 -0.770105	O 2.887853 -1.325479 3.394486
C -4.108765 1.212692 0.270334	C 1.861616 -1.981451 4.074177
C -2.985192 1.338999 -0.645743	H 2.176178 -2.205988 5.125616
H -3.954450 0.845632 1.293866	C 0.581438 -1.139015 4.104517
H -5.113824 1.517533 -0.052493	H -0.221739 -1.614024 4.702767
H -1.993183 1.323024 -0.157428	H 0.805019 -0.146513 4.545010
C -3.066918 2.213194 -1.869313	H 0.198031 -0.987336 3.076618
H -2.907871 3.263691 -1.550747	C 1.714709 -3.300261 3.303999
H -2.288730 1.942011 -2.609402	H 2.654952 -3.881153 3.317423
H -4.065770 2.128917 -2.342050	H 1.364503 -3.115845 2.270198
I -3.522454 3.890796 1.674866	I 0.187730 -4.743664 4.145468
O -3.289830 -1.253855 2.148873	O 4.423577 1.387755 1.988245
C -3.154934 -1.350505 3.541666	C 4.454607 2.700977 1.527199
H -2.258214 -0.766291 3.869463	H 3.591286 3.285193 1.938917
C -4.394377 -0.791499 4.240868	C 5.762123 3.391867 1.926990
H -4.301158 -0.838353 5.344852	H 5.799887 4.447055 1.586482
H -4.538564 0.267573 3.947229	H 5.859544 3.371911 3.031350
H -5.293754 -1.364854 3.930385	H 6.626857 2.842221 1.497938
C -2.885527 -2.837861 3.802759	C 4.251061 2.564427 0.013025
H -2.023465 -3.191583 3.205472	H 3.306173 2.038445 -0.217904
H -3.776569 -3.462424 3.593800	H 5.105448 2.055099 -0.474676
I -2.330333 -3.316621 5.924560	I 4.048240 4.517570 -1.105703
I_{BC} (X = I)	**C** (X = I)
SCF Done: -4246.31545504 A.U.	SCF Done: -4246.32728940 A.U.
Si -2.265990 1.506787 -1.817856	Si -2.757940 1.897356 -1.645154
Si -4.998955 -1.550825 -0.071683	Si -5.542602 -0.610723 0.498935
Si -2.286302 -2.783137 0.854248	Si -3.172952 -2.655669 0.372300
Si -0.828903 3.258910 0.405095	Si -0.325477 2.853183 0.039892
Si -5.739365 1.382724 0.993700	Si -4.949690 2.110845 2.198985
Si -0.597846 -1.072138 -1.012220	Si -1.640903 -1.079697 -1.725032
Si -2.876750 1.958669 2.206800	Si -1.836514 1.755780 2.399041
O -2.086396 3.247725 1.517769	O -1.212568 2.978108 1.462052
O -5.555366 -0.263197 0.822101	O -5.365580 0.618217 1.596530
O -1.411121 0.070299 -1.895863	O -2.353623 0.354693 -2.145407
O -4.500055 2.067640 1.857445	O -3.405902 2.127927 2.810649
O -3.920679 -2.469582 0.807132	O -4.573450 -1.912736 0.879549
O -1.622874 -2.343175 -0.622022	O -2.822557 -2.143419 -1.184460
O -1.413379 2.721947 -1.077718	O -1.429384 2.803290 -1.233771
O -1.535133 -1.927392 2.068460	O -1.891082 -2.278781 1.361441
O -0.057807 -0.418274 0.421340	O -0.541115 -0.879554 -0.485102
O -2.310172 0.554059 1.501492	O -1.875843 0.381188 1.455876
H -3.554977 1.274242 -1.094384	H -3.701113 1.806266 -0.487636
H -4.364313 -1.074029 -1.341231	H -5.227450 -0.130028 -0.883605
H 0.530390 -1.578616 -1.826092	H -0.977444 -1.650674 -2.919289
H -6.181715 -2.428027 -0.347654	H -6.960427 -1.083408 0.601589

H -5.839014 2.021768 -0.359995	H -5.099610 3.141780 1.119643
H -2.515079 1.922761 -3.231389	H -3.410872 2.561068 -2.815413
H -0.373177 4.660961 0.224195	H 0.476816 4.094288 -0.136420
H -6.996068 1.603257 1.777397	H -5.871416 2.398338 3.342676
H 0.237599 2.298322 0.795694	H 0.469798 1.597796 -0.011874
H -2.107522 -4.236492 1.091298	H -3.402944 -4.120991 0.393342
H -2.721177 1.977144 3.680484	H -1.083218 1.568916 3.659738
Si -0.944237 -0.365429 1.861153	Si -0.889530 -0.941362 1.168158
O -0.078883 0.244270 3.064514	O 0.431770 -0.977058 2.076436
Y 1.810068 1.300799 2.983584	Y 2.284267 -0.165861 2.726527
Cl 1.239734 3.799964 3.125816	Cl 1.995282 2.392477 2.499564
O 2.767217 1.221909 1.026860	O 3.441151 0.093146 0.635333
C 3.009436 2.092468 -0.057618	C 3.327017 0.844375 -0.601277
H 2.628283 3.109225 0.209509	H 2.734436 1.726722 -0.281895
C 4.509986 2.183434 -0.346878	C 4.695680 1.281987 -1.109995
H 4.728803 2.886159 -1.176439	H 4.581711 1.930170 -2.001863
H 5.034079 2.539577 0.562902	H 5.215726 1.861965 -0.321764
H 4.909451 1.182388 -0.610961	H 5.309153 0.399531 -1.374568
C 2.170480 1.562286 -1.229632	C 2.494696 -0.008363 -1.557068
H 1.116557 1.435407 -0.927506	H 1.575261 -0.381818 -1.065373
H 2.569472 0.619577 -1.644297	H 3.080235 -0.837165 -1.994448
I 2.075185 2.964770 -2.969074	I 1.720278 1.172884 -3.277605
C 2.944367 -0.868812 0.937781	C 4.095304 -1.225797 0.725985
O 3.310452 -1.138489 -0.154233	O 4.679971 -1.689980 -0.233784
O 2.611463 -1.050781 2.076346	O 3.869862 -1.635903 1.917646
O 3.117127 0.898740 4.554070	O 2.471604 -0.306115 4.793267
C 4.087457 0.205090 5.270343	C 2.459916 0.291944 6.054552
H 4.507333 0.853510 6.082025	H 2.477089 -0.492748 6.853186
C 3.510831 -1.069628 5.898661	C 3.667512 1.220045 6.234767
H 4.263962 -1.619206 6.500023	H 3.690307 1.689730 7.239380
H 2.661748 -0.798159 6.558193	H 4.600349 0.635724 6.097193
H 3.124949 -1.742053 5.103343	H 3.640626 2.020814 5.465257
C 5.191111 -0.059098 4.236882	C 1.108930 1.020115 6.105755
H 5.535671 0.882437 3.772488	H 0.275404 0.320438 5.911592
H 4.858914 -0.777576 3.463518	H 1.077191 1.869717 5.394484
I 7.090659 -0.962120 5.074707	I 0.598634 1.915229 8.117840
I_{CD} (X = I)	**D** (X = I)
SCF Done: -4246.30295432 A.U.	SCF Done: -4246.31678841 A.U.
Si -2.468006 1.589514 -2.080830	Si -0.210438 1.142366 -1.129242
Si -5.135476 -0.628046 -0.071633	Si -4.344985 0.569935 0.050959
Si -2.856762 -2.599223 0.584015	Si -3.997014 -2.479417 -0.402021
Si -0.666623 3.311528 -0.059800	Si 1.251464 0.434940 1.697069
Si -4.303937 1.935572 1.562365	Si -2.308619 1.995192 1.967311
Si -1.145326 -1.288474 -1.471489	Si -1.395975 -1.684366 -1.622247
Si -1.342831 2.006346 2.548369	Si -1.080264 -0.574884 3.226924
O -0.971843 3.321137 1.589656	O 0.531959 -0.770399 2.679251
O -4.303094 0.738597 0.395171	O -2.887740 1.123548 0.664063
O -2.156949 -0.030706 -1.841574	O -1.175655 -0.046131 -1.791864
O -3.000963 1.797008 2.585228	O -1.490243 1.025750 3.058522
O -4.414412 -2.010924 0.524542	O -4.568830 -1.067986 0.284333
O -2.145372 -2.529577 -0.926494	O -3.031000 -2.043026 -1.703986
O -1.928643 2.505614 -0.795116	O 0.208956 0.782695 0.448002
O -1.956953 -1.665950 1.625664	O -3.077720 -3.341717 0.691188
O -0.117189 -0.905848 -0.208505	O -0.844808 -2.128335 -0.122171
O -0.634086 0.691097 1.853565	O -2.045115 -1.486329 2.251714
H -3.953017 1.743128 -2.142566	H -0.982480 2.419672 -1.140623
H -5.167855 -0.660887 -1.564548	H -4.347253 0.880632 -1.410390
H -0.377372 -1.777067 -2.635955	H -0.693627 -2.401970 -2.712780
H -6.519205 -0.590517 0.508074	H -5.457629 1.257135 0.782798
H -4.295083 3.259285 0.867919	H -1.364784 3.037322 1.468465
H -1.832390 2.053300 -3.350133	H 1.048875 1.244581 -1.933173
H -0.666150 4.742919 -0.497724	H 1.389803 1.669259 2.527071
H -5.534302 1.771037 2.406275	H -3.469766 2.607942 2.693404
H 0.632312 2.645532 -0.353682	H 2.555836 -0.071336 1.205012
H -2.945986 -4.008796 1.038038	H -5.134987 -3.312274 -0.855220
H -0.887196 2.239537 3.935529	H -1.150149 -0.941783 4.655652
Si -0.474785 -0.904276 1.439842	Si -1.600232 -2.761342 1.242185
O 0.681851 -1.606104 2.327388	O -0.588563 -3.757063 1.999779
Y 2.501255 -0.928228 3.157486	Y 1.409595 -3.319196 2.644144
Cl 2.442600 1.522192 3.843463	Cl 2.513118 -5.498464 3.264346
O 2.938959 -0.108355 0.804144	O 2.917386 -1.999468 4.447451

C 2.684631 0.688289 -0.409778	C 3.936555 -1.049581 5.002191
H 1.593627 0.855237 -0.390049	H 4.915385 -1.555409 4.921617
C 3.466439 1.984911 -0.301753	C 3.884128 0.235467 4.205395
H 3.206888 2.636930 -1.158267	H 4.672852 0.909763 4.598739
H 3.202060 2.497969 0.643448	H 4.083960 0.037080 3.134139
H 4.558874 1.789313 -0.313516	H 2.897012 0.731588 4.313879
C 3.057279 -0.214682 -1.576897	C 3.468260 -0.948510 6.469530
H 2.381036 -1.037206 -1.837693	H 4.034793 -1.599389 7.160006
H 3.810521 0.085619 -2.311629	H 3.454367 0.081310 6.863529
I 1.363930 1.213240 -3.423929	I 6.671633 0.256819 6.949257
C 3.840841 -1.123028 0.609454	C 1.868808 -2.076534 5.290721
O 4.240245 -1.288078 -0.582545	O 2.061130 -1.437356 6.423707
O 4.125088 -1.764964 1.656504	O 0.855105 -2.694321 4.953413
O 2.834057 -1.898936 4.954845	O 2.478593 -2.616488 1.033885
C 2.988560 -1.939483 6.342329	C 3.261585 -2.381260 -0.094321
H 2.856101 -2.987245 6.713778	H 3.891450 -1.466542 0.060608
C 4.376519 -1.432965 6.751610	C 4.178395 -3.570668 -0.389600
H 4.537206 -1.483409 7.847937	H 4.827983 -3.384692 -1.268840
H 5.151152 -2.050507 6.252900	H 4.820185 -3.766943 0.492135
H 4.504926 -0.380585 6.419197	H 3.569149 -4.480252 -0.575563
C 1.831483 -1.079613 6.870306	C 2.247062 -2.079865 -1.204567
H 0.857433 -1.463118 6.514850	H 1.561381 -1.275242 -0.886383
H 1.954413 -0.015076 6.588747	H 1.661360 -2.977757 -1.478359
I 1.610206 -1.072063 9.114632	I 3.145078 -1.332282 -3.114038
Model B3:	
Y (X = Br)	**Y-PO** (X = Br)
SCF Done: -4301.81160802 A.U.	SCF Done: -4494.83923070 A.U.
Si -4.306032 2.123033 -1.034416	Si -3.933041 2.097841 -1.493355
Si -2.613902 -1.244233 0.883350	Si -2.539615 -1.135579 0.893361
Si -1.278239 -1.746617 -1.807446	Si -0.863566 -1.953094 -1.554224
Si -2.956449 2.561337 1.822896	Si -2.837576 2.784976 1.408814
Si -0.088912 -0.907901 2.686628	Si -0.156513 -0.730791 2.857298
Si -2.308579 0.791528 -3.216343	Si -1.782600 0.408648 -3.292203
Si 0.059970 1.801875 1.152195	Si 0.199448 1.883680 1.179716
O -1.315838 2.273010 1.935941	O -1.238973 2.460760 1.756008
O -1.669424 -1.263290 2.247819	O -1.741311 -0.908716 2.332979
O -3.322057 1.723976 -2.316665	O -2.908720 1.377749 -2.584635
O 0.502602 0.274651 1.647377	O 0.591644 0.456858 1.933149
O -1.899641 -2.166535 -0.333962	O -1.640448 -2.146713 -0.103028
O -2.345339 -0.789977 -2.649036	O -1.846558 -1.123343 -2.614204
O -3.417716 2.737771 0.232349	O -3.095406 2.804628 -0.238325
O 0.119003 -0.789902 -1.569067	O 0.510476 -0.974238 -1.323588
O -0.727038 1.318079 -3.061501	O -0.242701 1.003932 -3.021911
O -0.271742 1.722603 -0.477992	O 0.004569 1.589681 -0.446374
H -5.049164 0.900350 -0.583320	H -4.875040 1.065045 -0.949499
H -2.716597 0.150266 0.353247	H -2.685211 0.175991 0.190836
H -2.705831 0.838760 -4.639017	H -2.037411 0.336737 -4.747265
H -3.937146 -1.833713 1.224761	H -3.854372 -1.774232 1.182469
H -0.129453 -0.414580 4.092251	H -0.230224 -0.314939 4.286082
H -5.224870 3.196917 -1.513437	H -4.654144 3.182486 -2.224433
H -3.691224 1.413193 2.447339	H -3.698635 1.739964 2.051381
H 0.755130 -2.119310 2.491175	H 0.586109 -2.001562 2.628524
H -3.230206 3.844670 2.534081	H -3.136525 4.147960 1.942013
H -0.888348 -2.967117 -2.543192	H -0.449026 -3.273512 -2.064023
H 1.160823 2.754099 1.426738	H 1.282134 2.867971 1.415400
Si 0.302637 0.950992 -1.817120	Si 0.687471 0.724287 -1.672880
O 1.895540 0.980421 -2.080857	O 2.289258 0.787971 -1.854573
Y 2.427096 -1.115162 -1.875273	Y 2.881852 -1.334889 -1.685091
Cl 2.481536 -2.657366 -3.849003	Cl 2.371442 -2.915308 -3.601769
O 3.300156 -1.677969 -0.133740	O 3.411250 -2.018280 0.159938
C 3.605756 -1.848185 1.226645	C 3.500435 -2.201655 1.545699
H 2.780296 -2.421594 1.713921	H 2.564056 -2.685787 1.918394
C 4.915269 -2.612733 1.417266	C 4.693220 -3.083278 1.917809
H 5.144691 -2.722958 2.496686	H 4.766298 -3.198334 3.018354
H 4.843967 -3.621414 0.963877	H 4.586791 -4.087135 1.460383
H 5.751718 -2.068623 0.929728	H 5.634309 -2.627558 1.542850
C 3.625929 -0.452943 1.875195	C 3.569064 -0.802746 2.182016
H 2.762796 0.134354 1.515153	H 2.778626 -0.156163 1.759186
H 4.570473 0.087853 1.664273	H 4.563660 -0.336903 2.028166
Cl 3.440424 -0.548516 3.681250	Cl 3.261115 -0.846109 3.975855
	O 4.909241 -0.507603 -2.563080

	C 5.295021 0.899709 -2.626240 C 5.129052 0.126534 -3.875921 H 6.303540 1.094695 -2.223142 H 4.482429 1.583810 -2.321316 H 6.047999 -0.272738 -4.343961 C 3.930889 0.278197 -4.773075 H 4.194122 0.934296 -5.628480 H 3.618535 -0.708516 -5.171469 H 3.080137 0.729370 -4.224533
$\mathbf{I}_{AB}$ (X = Br)	**B** (X = Br)
SCF Done: -4508.38055158 A.U. Si 3.723375 -0.294865 0.223296 Si 0.564875 2.548689 -0.363728 Si -0.113224 -0.213942 -1.903615 Si 3.796132 -1.907958 2.912171 Si -0.596629 1.535230 2.475191 Si 2.160004 -2.220689 -1.693180 Si 0.856389 -1.149144 3.170244 O 2.452444 -1.256038 3.655985 O 0.360697 1.979615 1.170771 O 3.427831 -1.506590 -0.901054 O 0.336645 0.400843 3.330408 O 0.283831 1.320443 -1.482168 O 1.239877 -1.033575 -2.436954 O 4.311423 -0.965296 1.631257 O -0.744406 -1.080695 -0.593040 O 1.151793 -3.035902 -0.642663 O 0.868771 -1.600372 1.556006 H 2.481550 0.482960 0.498697 H 2.003505 2.938231 -0.522294 H 2.699770 -3.159128 -2.703205 H -0.361758 3.668148 -0.696279 H -0.770717 2.651251 3.434969 H 4.818698 0.557193 -0.332098 H 4.902209 -1.906745 3.917508 H -1.796878 0.790822 2.006260 H 3.502666 -3.294283 2.420412 H -1.124960 -0.195007 -2.986097 H 0.043044 -2.079074 3.991148 Si 0.005486 -2.333257 0.350418 O -1.281620 -3.193416 0.770615 Y -3.029163 -1.944812 0.231988 Cl -4.762376 -3.554171 -0.674651 O -3.665869 0.019053 -0.768290 C -3.994988 1.302290 0.296641 C -2.974168 1.297815 -0.736200 H -3.778016 0.923250 1.303423 H -4.997797 1.689824 0.068704 H -1.941781 1.208252 -0.351122 C -3.105331 2.158955 -1.965180 H -2.813013 3.193029 -1.691793 H -2.445942 1.800329 -2.780215 H -4.153390 2.164163 -2.325779 Br -2.993717 3.702902 1.445710 O -3.391336 -1.269885 2.141663 C -3.162485 -1.366712 3.519947 H -2.264167 -0.757742 3.796385 C -4.360666 -0.845067 4.314336 H -4.185733 -0.948822 5.404636 H -4.533314 0.224450 4.079419 H -5.272986 -1.416081 4.038958 C -2.827640 -2.837973 3.813036 H -2.008101 -3.178176 3.149797 H -3.716406 -3.482141 3.653108 Cl -2.272235 -3.104628 5.529078	SCF Done: -4508.41471719 A.U. Si -2.336706 1.923275 -0.919888 Si -3.321098 -1.241276 1.895737 Si -0.970253 -2.636990 0.324076 Si 0.349413 3.558504 -0.466555 Si -2.505584 1.511318 3.430184 Si -0.886565 -0.674137 -1.996215 Si 0.353919 1.905964 2.090906 O 0.471902 3.303148 1.186093 O -2.784945 -0.034917 2.898438 O -1.939561 0.603561 -1.863357 O -0.974585 2.036790 3.076115 O -2.089154 -2.283169 1.498292 O -1.487845 -1.977194 -1.130304 O -1.181474 3.114044 -0.994906 O 0.514642 -1.981666 0.685586 O 0.615680 -0.286225 -1.393601 O 0.114056 0.638345 1.039350 H -2.555849 1.499098 0.495429 H -3.909687 -0.648223 0.650026 H -0.788960 -1.031996 -3.432093 H -4.340196 -2.034329 2.652164 H -3.506112 2.438153 2.801574 H -3.590103 2.490745 -1.507245 H 0.463455 5.024178 -0.711964 H -2.646360 1.510637 4.920063 H 1.359095 2.744409 -1.205599 H -0.863617 -4.109757 0.212530 H 1.557063 1.762740 2.940222 Si 1.084035 -0.462784 0.214258 O 2.653382 -0.272983 0.469774 Y 3.996931 -0.438484 2.153193 Cl 5.616780 -2.394120 1.863881 O 2.673092 -0.793214 3.739306 C 1.713133 -1.612592 4.338501 H 1.963860 -1.780548 5.417739 C 0.313518 -0.996796 4.245011 H -0.446429 -1.612353 4.766617 H 0.322397 0.014880 4.697518 H 0.009072 -0.908110 3.183600 C 1.832865 -2.947070 3.593276 H 2.842533 -3.385002 3.698134 H 1.553430 -2.830866 2.528440 Br 0.566498 -4.416600 4.280873 O 4.909209 1.452478 2.267743 C 5.128469 2.608212 1.517708 H 5.532262 3.428784 2.167250 C 6.119633 2.368115 0.371257 H 6.291890 3.291937 -0.218895 H 7.087443 2.014411 0.781120 H 5.727083 1.583343 -0.311809 C 3.741887 3.044369 1.017330 H 3.070414 3.229057 1.874161 H 3.307956 2.251929 0.373473 Cl 3.721484 4.586380 0.028627
$\mathbf{I}_{BC}$ (X = Br)	**C** (X = Br)
SCF Done: -4696.88031832 A.U. Si -2.662587 1.686322 -1.881513 Si -5.517139 -0.971129 0.026115 Si -2.975384 -2.735443 0.510326 Si -0.631044 3.023681 0.081764	SCF Done: -4696.89349826 A.U. Si -2.726347 1.895342 -1.672745 Si -5.512500 -0.629357 0.452464 Si -3.141402 -2.671872 0.363550 Si -0.323354 2.846642 0.037298

Si -5.567469 1.925836 1.470550	Si -4.966352 2.089093 2.170335
Si -1.302751 -1.161992 -1.465376	Si -1.594273 -1.082066 -1.709476
Si -2.501856 1.984212 2.205617	Si -1.853773 1.771337 2.394909
O -1.765032 3.176179 1.314947	O -1.244888 2.985221 1.437373
O -5.689291 0.318629 1.056980	O -5.352809 0.590322 1.563493
O -2.109858 0.126305 -2.120216	O -2.324135 0.341271 -2.137166
O -4.142872 2.270908 2.246404	O -3.429294 2.133600 2.797229
O -4.520318 -2.137637 0.677211	O -4.557619 -1.938822 0.842750
O -2.408897 -2.343272 -1.018580	O -2.768951 -2.164796 -1.189934
O -1.483832 2.717539 -1.339902	O -1.400617 2.805795 -1.261272
O -1.948434 -2.098804 1.651524	O -1.882889 -2.280571 1.376461
O -0.460422 -0.722710 -0.095622	O -0.520061 -0.874599 -0.449977
O -2.273138 0.533079 1.412749	O -1.880427 0.378587 1.479827
H -3.803714 1.652448 -0.913744	H -3.683804 1.829245 -0.524506
H -4.988274 -0.521673 -1.300081	H -5.167148 -0.139400 -0.919283
H -0.376016 -1.714781 -2.481139	H -0.899029 -1.638868 -2.892502
H -6.871592 -1.597085 -0.113197	H -6.934164 -1.097135 0.522464
H -5.713586 2.771764 0.239978	H -5.124495 3.118243 1.090372
H -3.115929 2.178212 -3.219208	H -3.363533 2.539206 -2.862805
H 0.059321 4.328303 -0.096550	H 0.494882 4.078470 -0.129259
H -6.671138 2.211574 2.441842	H -5.903498 2.360885 3.305829
H 0.273016 1.867467 0.318128	H 0.449073 1.578608 0.010304
H -3.042166 -4.209235 0.668078	H -3.361046 -4.138858 0.386863
H -2.020699 1.964217 3.606335	H -1.101523 1.617369 3.660881
Si -1.090965 -0.659121 1.475019	Si -0.884319 -0.938008 1.199767
O 0.033534 -0.399116 2.584616	O 0.430610 -0.968533 2.116411
Y 1.930133 0.582137 2.878588	Y 2.286942 -0.138829 2.745978
Cl 1.338679 3.080955 2.885852	Cl 1.961976 2.417079 2.493484
O 3.106603 0.598972 1.059870	O 3.428086 0.130066 0.636201
C 3.154026 1.410847 -0.091504	C 3.272875 0.859590 -0.606085
H 2.619937 2.371766 0.113425	H 2.672056 1.737382 -0.290052
C 4.596196 1.724342 -0.493979	C 4.615479 1.314143 -1.164684
H 4.628103 2.357735 -1.404515	H 4.453293 1.932714 -2.070422
H 5.102173 2.265536 0.330905	H 5.145508 1.929597 -0.410753
H 5.152316 0.784434 -0.690105	H 5.241067 0.438647 -1.424281
C 2.362538 0.649738 -1.160336	C 2.429800 -0.009469 -1.537103
H 1.390664 0.311750 -0.756512	H 1.547700 -0.422467 -1.012021
H 2.928688 -0.200484 -1.584190	H 3.018434 -0.805223 -2.026949
Br 1.868039 1.815466 -2.758901	Br 1.620813 1.097672 -3.032887
C 3.591813 -1.532612 1.072007	C 4.077565 -1.190258 0.717407
O 4.237498 -1.706875 0.099402	O 4.642253 -1.657287 -0.253707
O 3.008341 -1.736221 2.094954	O 3.873546 -1.599684 1.912852
O 2.930994 0.215282 4.664588	O 2.479837 -0.271082 4.801412
C 4.029620 0.057175 5.498939	C 2.436962 0.293136 6.075324
H 3.759577 -0.563716 6.393689	H 2.350303 -0.509135 6.853572
C 5.202433 -0.621013 4.777331	C 3.694781 1.121611 6.364749
H 6.080490 -0.734925 5.445834	H 3.655846 1.575145 7.376425
H 4.890944 -1.620707 4.413221	H 4.593723 0.475677 6.293052
H 5.503419 -0.013189 3.895854	H 3.787174 1.934740 5.612904
C 4.389132 1.462507 6.013605	C 1.150557 1.137317 6.131174
H 3.503276 1.927730 6.485712	H 0.275389 0.504482 5.887487
H 4.732408 2.105176 5.177471	H 1.209637 1.973892 5.405611
Cl 5.720023 1.456514 7.268360	Cl 0.830849 1.862392 7.778011
I_{cp} (X = Br)	**D** (X = Br)
SCF Done: -4696.87058069 A.U.	SCF Done: -4696.87671115 A.U.
Si -2.358058 1.592111 -2.121795	Si -3.775519 -0.018321 -1.029124
Si -5.118300 -0.609142 -0.211710	Si -1.885866 -3.877429 1.094352
Si -2.872532 -2.603559 0.519916	Si -0.078004 -3.708259 -1.430175
Si -0.672879 3.378939 -0.027323	Si -3.543673 -0.316400 2.145311
Si -4.339897 1.938511 1.481365	Si 0.278951 -2.542530 2.986726
Si -1.101028 -1.301681 -1.482715	Si -1.833501 -1.647776 -2.860343
Si -1.405508 1.966291 2.522427	Si -0.468151 0.162925 1.713147
O -1.031493 3.311709 1.610336	O -2.003334 0.301205 2.330833
O -4.330119 0.771853 0.286321	O -1.188074 -3.084760 2.385143
O -2.104751 -0.029738 -1.826708	O -3.201299 -1.248209 -2.003767
O -3.064784 1.753227 2.531988	O 0.434500 -0.920167 2.588881
O -4.415793 -1.980977 0.429045	O -0.708759 -4.310947 -0.015706
O -2.126512 -2.540896 -0.973317	O -1.330019 -3.174937 -2.402661
O -1.851487 2.528188 -0.839041	O -3.929904 -0.550258 0.543900
O -1.977869 -1.703884 1.595471	O 0.860786 -2.343252 -1.072070
O -0.085068 -0.976907 -0.194274	O -0.609841 -0.570901 -2.486734

O -0.685230 0.674810 1.794663	O -0.639486 -0.388140 0.147475
H -3.838128 1.772842 -2.235335	H -5.153392 0.303647 -1.514594
H -5.081643 -0.648641 -1.704053	H -2.888070 -2.973392 0.460401
H -0.333388 -1.784659 -2.649632	H -2.121888 -1.624877 -4.311351
H -6.528708 -0.584705 0.301768	H -2.501084 -5.142889 1.602706
H -4.290254 3.276722 0.816258	H 0.220255 -2.676737 4.470576
H -1.682407 2.015162 -3.383553	H -2.868393 1.169597 -1.092692
H -0.754252 4.823466 -0.415580	H -3.669977 -1.633101 2.839437
H -5.593361 1.779551 2.292185	H 1.390486 -3.311497 2.356161
H 0.681695 2.819325 -0.285590	H -4.476134 0.698016 2.733150
H -3.004773 -4.014031 0.961920	H 0.732317 -4.754587 -2.076593
H -0.972562 2.159382 3.923282	H 0.202620 1.481534 1.777059
Si -0.495524 -0.933876 1.440424	Si 0.372567 -0.683521 -1.140438
O 0.636666 -1.599662 2.384395	O 1.798988 0.045477 -1.181600
Y 2.454706 -0.910855 3.217723	Y 3.224519 -1.617901 -1.541878
Cl 2.350244 1.541186 3.902472	Cl 3.214629 -3.514708 -3.237995
O 2.900744 -0.067228 0.879679	O 4.056329 -2.199141 0.231816
C 2.602388 0.709837 -0.334087	C 4.212730 -2.479441 1.587974
H 1.517709 0.900470 -0.273241	H 3.553693 -3.336727 1.879540
C 3.415705 1.990634 -0.298867	C 5.661631 -2.842660 1.922852
H 3.135081 2.618672 -1.166584	H 5.778212 -3.039572 3.008404
H 3.200605 2.540490 0.638076	H 5.966167 -3.746547 1.358082
H 4.502328 1.769129 -0.346484	H 6.336953 -2.009507 1.633705
C 2.895347 -0.221471 -1.501684	C 3.713446 -1.246637 2.359409
H 2.195266 -1.038828 -1.706429	H 2.723160 -0.930817 1.982868
H 3.611415 0.053916 -2.282126	H 4.426242 -0.401567 2.277700
Br 1.232281 1.127868 -3.069322	Cl 3.481739 -1.591942 4.137935
C 3.759485 -1.113250 0.654608	O 3.090087 0.058839 -3.987342
O 4.101022 -1.295818 -0.553462	C 2.551352 1.109222 -4.916399
O 4.062864 -1.759829 1.692269	H 2.265456 0.589802 -5.847673
O 2.820586 -1.876579 5.001375	C 1.372771 1.788613 -4.252468
C 3.047833 -1.936895 6.375747	H 0.970959 2.521966 -4.981238
H 2.881540 -2.979267 6.752136	H 0.589550 1.049733 -3.995831
C 4.479905 -1.512956 6.723435	H 1.683912 2.308215 -3.322719
H 4.656662 -1.549139 7.817763	C 3.803184 1.982909 -5.122782
H 5.203917 -2.184434 6.218384	H 4.367019 1.743941 -6.042391
H 4.658505 -0.475274 6.368086	H 3.607776 3.066765 -5.079333
C 1.989250 -1.029829 7.028257	Br 2.144862 2.873691 -7.693081
H 0.975266 -1.363373 6.734707	C 4.205036 0.512747 -3.422430
H 2.134258 0.021093 6.704564	O 4.662946 1.627097 -3.949526
Cl 2.041723 -1.057091 8.853035	O 4.734983 -0.091402 -2.469233
I_{AB} (X = I)	**B** (X = I)
SCF Done: -4506.44380077 A.U.	SCF Done: -4506.47974303 A.U.
Si 3.709188 -0.302442 0.219489	Si -2.346245 1.926634 -0.702711
Si 0.601517 2.501779 -0.437243	Si -3.291578 -1.027964 2.402656
Si -0.121024 -0.266334 -1.921830	Si -1.307815 -2.534466 0.359349
Si 3.819287 -1.912354 2.911702	Si 0.429307 3.459748 -0.549840
Si -0.560792 1.538933 2.460461	Si -2.074341 1.761509 3.476257
Si 2.174279 -2.246579 -1.699336	Si -1.122567 -0.626705 -2.005745
Si 0.881760 -1.154515 3.175175	Si 0.731239 1.795194 1.959962
O 2.474972 -1.267054 3.663240	O 0.962219 3.145245 1.007962
O 0.309004 1.980373 1.097850	O -2.482776 0.171358 3.217331
O 3.434001 -1.507929 -0.915682	O -1.972111 0.797673 -1.880021
O 0.389352 0.412465 3.287232	O -0.520143 2.092747 3.011803
O 0.258616 1.285797 -1.545060	O -2.249200 -2.060721 1.634855
O 1.237604 -1.078404 -2.452855	O -1.853999 -1.788322 -1.042120
O 4.312611 -0.971045 1.621127	O -1.220993 3.145675 -0.640384
O -0.713631 -1.103437 -0.576405	O 0.279152 -2.095507 0.588293
O 1.180209 -3.061336 -0.635003	O 0.452822 -0.434825 -1.506563
O 0.886860 -1.644565 1.574946	O 0.276439 0.544358 0.960027
H 2.449674 0.443828 0.505474	H -2.462270 1.249019 0.622468
H 2.062029 2.811229 -0.563914	H -4.229925 -0.415748 1.402626
H 2.723335 -3.188466 -2.700503	H -1.164190 -1.043489 -3.428334
H -0.245950 3.673897 -0.805310	H -4.038826 -1.830899 3.419664
H -0.698158 2.696617 3.377945	H -3.030150 2.649912 2.732541
H 4.781452 0.580777 -0.330522	H -3.645454 2.552891 -1.099283
H 4.932490 -1.894503 3.908302	H 0.584310 4.919089 -0.808250
H -1.808424 0.842150 2.043593	H -2.159577 2.012096 4.949355
H 3.532153 -3.303096 2.430078	H 1.128468 2.588900 -1.541206
H -1.151112 -0.281538 -2.986043	H -1.414736 -4.005965 0.226731
H 0.051016 -2.040446 4.025329	H 1.965350 1.527638 2.728732

Si 0.030068 -2.367179 0.358126	Si 1.016958 -0.670606 0.063175
O -1.261376 -3.226490 0.765025	O 2.613886 -0.700564 0.189461
Y -2.990116 -1.948762 0.223646	Y 4.041200 -0.668471 1.808464
Cl -4.752098 -3.518283 -0.694497	Cl 6.114381 -2.099349 1.345976
O -3.559491 0.022952 -0.790013	O 2.886406 -1.316200 3.426923
C -4.110650 1.227755 0.255253	C 1.862276 -1.988118 4.093023
C -2.981381 1.352091 -0.654354	H 2.170231 -2.219040 5.145223
H -3.965738 0.849924 1.276597	C 0.572967 -1.159311 4.120862
H -5.112192 1.537899 -0.073422	H -0.231080 -1.648607 4.706373
H -1.992283 1.330821 -0.159950	H 0.782650 -0.169198 4.573191
C -3.052263 2.232875 -1.874243	H 0.197378 -1.001293 3.090960
H -2.893822 3.281652 -1.549828	C 1.734042 -3.301761 3.310718
H -2.269417 1.963472 -2.610137	H 2.680754 -3.872069 3.323129
H -4.047781 2.152299 -2.354672	H 1.384298 -3.113546 2.277408
I -3.529487 3.900208 1.669466	I 0.221162 -4.771985 4.135423
O -3.337145 -1.250099 2.127488	O 4.464673 1.369885 1.972003
C -3.146802 -1.351157 3.511738	C 4.394625 2.667699 1.477322
H -2.268888 -0.725878 3.816780	H 3.519924 3.216780 1.914018
C -4.377106 -0.859398 4.274853	C 5.669485 3.458604 1.790351
H -4.230135 -0.965967 5.368994	H 5.619176 4.484897 1.371310
H -4.566915 0.207367 4.041357	H 5.808918 3.524780 2.888441
H -5.268420 -1.449104 3.971497	H 6.551420 2.935349 1.362707
C -2.790579 -2.817228 3.805932	C 4.129219 2.546556 -0.033520
H -1.955882 -3.143095 3.154554	H 3.245918 1.905872 -0.217890
H -3.664983 -3.476966 3.630830	H 5.005030 2.111005 -0.556443
Cl -2.257227 -3.077956 5.529325	Cl 3.775085 4.151023 -0.841621
I_{BC} (X = I)	**C** (X = I)
SCF Done: -4694.94291829 A.U.	SCF Done: -4694.95471815 A.U.
Si -2.173359 1.517888 -1.806531	Si -2.780883 1.898675 -1.649359
Si -5.170183 -1.365367 -0.234825	Si -5.538252 -0.633116 0.508235
Si -2.603684 -2.768536 0.838926	Si -3.162613 -2.665788 0.363061
Si -0.756534 3.168338 0.513954	Si -0.345597 2.858913 0.024662
Si -5.788160 1.607262 0.803579	Si -4.953300 2.084013 2.215445
Si -0.711543 -1.158937 -0.917557	Si -1.653645 -1.074542 -1.739200
Si -2.973563 1.990741 2.194480	Si -1.837964 1.750221 2.389487
O -2.060133 3.231128 1.570746	O -1.235759 2.978313 1.446037
O -5.699619 -0.046109 0.628673	O -5.365165 0.590166 1.613299
O -1.397815 0.035663 -1.839375	O -2.377961 0.356544 -2.152059
O -4.561331 2.207004 1.744641	O -3.406497 2.109983 2.818997
O -4.211178 -2.353235 0.705385	O -4.566189 -1.935014 0.881438
O -1.834764 -2.365076 -0.596422	O -2.826809 -2.146136 -1.194341
O -1.308476 2.677950 -0.997393	O -1.451469 2.807812 -1.248326
O -1.867719 -1.969711 2.099653	O -1.878077 -2.283596 1.345884
O -0.213913 -0.545529 0.547406	O -0.548531 -0.872145 -0.505245
O -2.454543 0.556538 1.514313	O -1.878227 0.375633 1.447097
H -3.521132 1.355478 -1.176880	H -3.715956 1.806312 -0.485149
H -4.425493 -0.929543 -1.457997	H -5.224890 -0.143400 -0.871380
H 0.426534 -1.734212 -1.670226	H -0.996059 -1.639256 -2.939630
H -6.387197 -2.163602 -0.590601	H -6.955043 -1.109846 0.608699
H -5.767291 2.258523 -0.547778	H -5.116771 3.116321 1.139370
H -2.299933 1.955806 -3.229761	H -3.444368 2.560523 -2.814970
H -0.206455 4.539340 0.361644	H 0.450581 4.104065 -0.151149
H -7.072961 1.903582 1.513522	H -5.869957 2.364026 3.365448
H 0.227951 2.138960 0.941683	H 0.452668 1.606111 -0.031070
H -2.530787 -4.231844 1.072178	H -3.383171 -4.132760 0.380801
H -2.912745 1.992243 3.675430	H -1.070834 1.570536 3.643035
Si -1.167622 -0.446772 1.941594	Si -0.884005 -0.940025 1.150670
O -0.329771 0.100818 3.192900	O 0.441970 -0.969757 2.050313
Y 1.628604 1.050486 3.169073	Y 2.280353 -0.142971 2.731674
Cl 1.246779 3.591394 3.276611	Cl 1.975922 2.414177 2.468729
O 2.657171 0.939689 1.247863	O 3.454031 0.115887 0.643390
C 3.007734 1.802155 0.186067	C 3.329348 0.853598 -0.599622
H 2.670111 2.836009 0.444542	H 2.733816 1.736091 -0.285766
C 4.524167 1.810215 -0.021131	C 4.692566 1.293319 -1.121136
H 4.825046 2.497764 -0.837500	H 4.569868 1.931815 -2.018876
H 5.017671 2.141521 0.914742	H 5.213885 1.883970 -0.341698
H 4.882518 0.788430 -0.263253	H 5.309220 0.411316 -1.379801
C 2.200564 1.324272 -1.029768	C 2.496077 -0.013126 -1.542098
H 1.126678 1.264837 -0.783009	H 1.580185 -0.385119 -1.043022
H 2.561350 0.357396 -1.423325	H 3.083025 -0.843695 -1.974208
I 2.280526 2.725966 -2.770563	I 1.705443 1.145564 -3.270955

C 2.761026 -1.129636 1.159473	C 4.110202 -1.200736 0.742758
O 3.198581 -1.417841 0.097265	O 4.698349 -1.668903 -0.213535
O 2.335409 -1.311485 2.267502	O 3.883285 -1.605734 1.935609
O 2.927477 0.626875 4.736007	O 2.430718 -0.272479 4.791228
C 4.202061 0.264092 5.161067	C 2.402024 0.301398 6.061287
H 4.411997 0.694218 6.175352	H 2.300010 -0.493290 6.845412
C 4.364596 -1.259433 5.234587	C 3.677706 1.105267 6.342578
H 5.386613 -1.540431 5.562413	H 3.651004 1.565968 7.351385
H 3.626945 -1.680220 5.947633	H 4.562683 0.440128 6.272715
H 4.167923 -1.705312 4.237042	H 3.785079 1.911653 5.585426
C 5.189776 0.914129 4.174250	C 1.134141 1.173144 6.113057
H 5.020148 2.007599 4.137712	H 0.244888 0.557326 5.877101
H 5.054244 0.490143 3.157971	H 1.209410 2.001885 5.380128
Cl 6.947237 0.671365 4.618638	Cl 0.834301 1.918963 7.754497
I_{CD} (X = I)	**D** (X = I)
SCF Done: -4694.93067004 A.U.	SCF Done: -4694.94544403 A.U.
Si -2.459900 1.578448 -2.115322	Si -0.161861 1.115309 -1.134542
Si -5.156121 -0.615801 -0.128293	Si -4.333175 0.575246 0.047456
Si -2.891741 -2.595698 0.563805	Si -3.987686 -2.476734 -0.406223
Si -0.688545 3.318430 -0.088170	Si 1.257007 0.430839 1.705532
Si -4.334342 1.944933 1.515895	Si -2.286512 1.999790 1.952559
Si -1.150033 -1.304965 -1.473652	Si -1.392655 -1.678952 -1.630321
Si -1.377261 2.003007 2.515010	Si -1.078283 -0.575539 3.225853
O -1.001909 3.318939 1.559621	O 0.537313 -0.771566 2.689191
O -4.333873 0.756163 0.340504	O -2.873467 1.131945 0.650303
O -2.148665 -0.035560 -1.839672	O -1.175497 -0.038137 -1.788404
O -3.036428 1.795793 2.543419	O -1.486374 1.025372 3.052772
O -4.443914 -1.994367 0.487289	O -4.553226 -1.063279 0.280664
O -2.166129 -2.538530 -0.940702	O -3.025895 -2.043390 -1.713403
O -1.948566 2.521517 -0.837606	O 0.207480 0.782736 0.461523
O -1.994305 -1.667614 1.611151	O -3.068355 -3.341874 0.684369
O -0.124119 -0.940552 -0.204491	O -0.841849 -2.127071 -0.131833
O -0.667281 0.688285 1.821262	O -2.037251 -1.487066 2.245149
H -3.943753 1.727420 -2.208093	H -0.872887 2.426693 -1.192154
H -5.167530 -0.657806 -1.621292	H -4.347642 0.886533 -1.413817
H -0.381413 -1.793132 -2.638105	H -0.686103 -2.384207 -2.726661
H -6.548278 -0.576144 0.431072	H -5.442729 1.259496 0.787038
H -4.318926 3.272969 0.829856	H -1.330713 3.030442 1.453025
H -1.800157 2.019039 -3.380600	H 1.117882 1.134572 -1.912838
H -0.684359 4.752858 -0.516265	H 1.402416 1.665756 2.533713
H -5.568773 1.779500 2.354023	H -3.442742 2.629087 2.672820
H 0.610126 2.652000 -0.381717	H 2.557492 -0.076892 1.205247
H -2.998680 -4.003058 1.021380	H -5.129267 -3.306342 -0.856674
H -0.930217 2.236301 3.904954	H -1.158898 -0.939921 4.654572
Si -0.504195 -0.915887 1.439349	Si -1.590035 -2.761474 1.236014
O 0.631989 -1.610170 2.356275	O -0.575140 -3.755031 1.990495
Y 2.448296 -0.924891 3.198962	Y 1.424294 -3.326642 2.649377
Cl 2.381444 1.535396 3.859368	Cl 2.497717 -5.516761 3.291202
O 2.892954 -0.116302 0.840711	O 2.909989 -2.021400 4.458262
C 2.660815 0.690214 -0.369284	C 3.932581 -1.073365 5.007351
H 1.568031 0.845850 -0.375415	H 4.908652 -1.585582 4.934100
C 3.426190 1.993851 -0.228331	C 3.890188 0.205177 4.199525
H 3.182214 2.653522 -1.083484	H 4.682263 0.878013 4.588599
H 3.133948 2.492831 0.716258	H 4.090070 -0.004280 3.130357
H 4.520452 1.808664 -0.214886	H 2.906028 0.708211 4.302589
C 3.071715 -0.194729 -1.537063	C 3.460207 -0.956904 6.472367
H 2.418793 -1.029801 -1.816355	H 4.020513 -1.605543 7.170042
H 3.839065 0.121155 -2.250184	H 3.452781 0.076409 6.857387
I 1.398185 1.209576 -3.408493	I 6.667977 0.248282 6.956648
C 3.822884 -1.109354 0.662955	C 1.856562 -2.084130 5.298157
O 4.255676 -1.257538 -0.519385	O 2.050460 -1.436366 6.426482
O 4.096531 -1.749487 1.713674	O 0.840451 -2.696504 4.960945
O 2.782555 -1.883414 4.991921	O 2.498336 -2.628140 1.048657
C 3.003041 -1.937209 6.367820	C 3.223343 -2.346813 -0.105586
H 2.822926 -2.975014 6.750206	H 3.805951 -1.396543 0.025229
C 4.438334 -1.527332 6.718929	C 4.198707 -3.474340 -0.450487
H 4.609588 -1.557116 7.814310	H 4.754407 -3.247987 -1.383350
H 5.156839 -2.210963 6.222432	H 4.922437 -3.614632 0.376994
H 4.630594 -0.494601 6.356409	H 3.641644 -4.425946 -0.582670
C 1.952156 -1.013818 7.009845	C 2.186964 -2.087162 -1.209594
H 0.935637 -1.336762 6.713197	H 1.459413 -1.338752 -0.848348

H 2.111585 0.033535 6.681372	H 1.639844 -3.016843 -1.460714
Cl 1.995537 -1.031664 8.834796	Cl 2.902196 -1.433383 -2.747940
Model B2, CO_2 insertion:	
Y-PO—CO_2 (X = Br)	**Y-PO—CO_2** (X = I)
SCF Done: -4043.60323900 A.U.	SCF Done: -4041.66534063 A.U.
Si 3.265556 -3.544158 -0.288857	Si 3.262940 -3.547377 -0.286490
Si 1.218220 1.221452 0.269200	Si 1.214662 1.217621 0.283100
Si 0.674988 -0.766886 -1.981214	Si 0.680020 -0.762114 -1.976769
Si 2.390863 -5.049015 2.446567	Si 2.382612 -5.065564 2.437536
Si 0.719056 -0.866043 2.422244	Si 0.707836 -0.877470 2.428218
Si 1.318369 -3.611831 -2.654271	Si 1.325417 -3.604257 -2.659929
Si -0.315624 -3.709981 2.069816	Si -0.321228 -3.722458 2.057755
O 1.069125 -4.087436 2.896037	O 1.062318 -4.101302 2.885506
O 0.193106 0.314821 1.320547	O 0.186686 0.306279 1.327175
O 2.366525 -4.236827 -1.526945	O 2.369821 -4.234340 -1.531993
O -0.513880 -2.015596 2.186450	O -0.521248 -2.028714 2.180015
O 1.566317 0.335944 -1.108959	O 1.568498 0.336817 -1.096555
O 1.596150 -1.951356 -2.715139	O 1.603667 -1.943524 -2.712421
O 3.155524 -4.428109 1.113682	O 3.153385 -4.443056 1.108740
O -0.185838 -1.595546 -0.777419	O -0.185761 -1.595426 -0.779959
O -0.286569 -3.854421 -2.176153	O -0.281111 -3.848623 -2.188234
O -0.040955 -4.046602 0.464848	O -0.042490 -4.052273 0.452130
H 2.760999 -2.161398 -0.022275	H 2.752321 -2.168661 -0.010245
H 2.506875 1.371285 1.014969	H 2.500346 1.367618 1.033831
H 1.518997 -4.244326 -3.973441	H 1.530431 -4.230768 -3.981278
H 0.550651 2.512148 -0.023808	H 0.545376 2.507796 -0.008652
H 2.046900 -1.403798 2.011549	H 2.039523 -1.410975 2.024617
H 4.701884 -3.555372 -0.692146	H 4.700286 -3.549508 -0.686284
H 3.333805 -5.005835 3.600227	H 3.322226 -5.028926 3.594135
H 0.673761 -0.356369 3.818554	H 0.649039 -0.374158 3.826412
H 1.897078 -6.426982 2.143770	H 1.885580 -6.441138 2.129059
H -0.162875 -0.118861 -3.007833	H -0.153574 -0.108863 -3.003565
H -1.521508 -4.343216 2.645638	H -1.527334 -4.359376 2.629000
Si -0.836449 -3.197393 -0.752947	Si -0.835381 -3.197806 -0.763846
O -2.336060 -2.834731 -0.286223	O -2.336278 -2.838084 -0.299324
Y -2.067430 -0.764507 0.519675	Y -2.071248 -0.770684 0.516140
Cl -1.961282 1.192521 -1.076623	Cl -1.966818 1.189362 -1.075854
O -2.914958 -0.069389 2.399008	O -2.918125 -0.066716 2.394752
C -2.520034 0.304415 3.707507	C -2.520083 0.328972 3.697723
H -1.437582 0.579720 3.674030	H -1.444797 0.628392 3.645231
C -3.299674 1.516927 4.214536	C -3.324162 1.531459 4.191363
H -2.927395 1.830510 5.210292	H -2.950421 1.880430 5.174657
H -3.172391 2.361011 3.507839	H -3.227215 2.361635 3.463689
H -4.379489 1.284972 4.294736	H -4.396798 1.274633 4.289607
C -2.659478 -0.952729 4.571991	C -2.629329 -0.929289 4.567115
H -2.176265 -1.811540 4.073517	H -2.125644 -1.775525 4.067221
H -3.714254 -1.183116 4.814409	H -3.679407 -1.187913 4.803280
Br -1.698481 -0.773186 6.345270	I -1.589142 -0.742948 6.527392
C -4.772336 -0.493886 1.836886	C -4.771626 -0.512928 1.842799
O -4.489524 -0.794670 0.694170	O -4.490453 -0.815836 0.699913
O -5.510323 -0.340916 2.745397	O -5.509221 -0.364715 2.752394
Y (X = Br)	**Y-PO** (X = Br)
SCF Done: -4043.60896689 A.U.	SCF Done: -4236.62224815 A.U.
Si -3.276975 2.663931 -0.778649	Si 4.225642 -0.395384 -0.604139
Si -3.026418 -1.676556 0.827351	Si 0.605335 2.491362 -0.462823
Si -1.511852 -1.993267 -1.906801	Si -0.240211 -0.277328 -1.853598
Si -2.502255 2.201520 2.237532	Si 4.668667 -2.174979 1.997489
Si -0.347663 -1.267961 2.389829	Si 0.974674 1.955503 2.652215
Si -2.371587 0.678962 -3.102554	Si 2.180692 -2.140390 -2.243430
Si 0.321649 1.388206 1.162873	Si 1.950582 -1.091644 2.686779
O -0.833970 2.021230 2.158776	O 3.508082 -1.549843 3.040776
O -1.894604 -0.947430 1.818868	O 0.298005 2.142456 1.131489
O -3.246037 1.465169 -1.944410	O 3.605015 -1.518946 -1.686444
O 0.697725 -0.180432 1.620919	O 1.860422 0.552182 2.766185
O -2.233739 -2.378815 -0.478879	O -0.044955 1.300312 -1.435893
O -2.461326 -0.967431 -2.806825	O 1.127298 -0.877764 -2.591208
O -3.197405 1.970257 0.737416	O 4.920093 -1.151861 0.702139
O -0.065958 -1.135603 -1.602988	O -0.470806 -1.248221 -0.485620
O -0.746195 1.100615 -2.993523	O 1.433042 -3.084195 -1.068896
O -0.321593 1.335133 -0.383538	O 1.714867 -1.582428 1.101456

H -4.602763 3.340058 -0.909071 H -3.972698 -0.627410 0.360529 H -2.877802 0.976996 -4.458337 H -3.692728 -2.797035 1.556372 H -0.331777 -0.979582 3.855443 H -2.137283 3.611141 -0.986963 H -3.079795 1.201745 3.177992 H 0.068297 -2.651057 2.043387 H -2.747389 3.605717 2.695269 H -1.170685 -3.228174 -2.643683 H 1.558649 2.199128 1.219735 Si 0.229894 0.588702 -1.757495 O 1.836227 0.528983 -1.912996 Y 2.280739 -1.556728 -1.574558 Cl 2.893765 -2.853219 -3.601666 O 3.015538 -2.434502 2.205470 C 4.042976 -1.707329 2.968599 H 3.766868 -1.976534 4.007497 C 5.442227 -2.217030 2.652030 H 6.169124 -1.732781 3.334280 H 5.500158 -3.312452 2.806071 H 5.724044 -1.978679 1.608215 C 3.842141 -0.200351 2.789557 H 2.767435 0.052291 2.757491 H 4.355467 0.202259 1.900324 Br 4.603547 0.797625 4.369687 C 2.892735 -2.244256 0.891826 O 3.674521 -1.451068 0.242493 O 1.937826 -2.852727 0.299980	H 3.137223 0.526354 -0.156579 H 2.076241 2.598802 -0.713303 H 2.431952 -2.961421 -3.446113 H -0.113823 3.751784 -0.820816 H 1.960782 3.065963 2.852506 H 5.315959 0.335474 -1.313880 H 5.943699 -2.249405 2.767306 H -0.124117 2.011159 3.654319 H 4.228372 -3.515705 1.495905 H -1.415786 -0.393054 -2.745535 H 1.009903 -1.753918 3.621681 Si 0.605644 -2.424962 0.207425 O -0.483178 -3.269512 1.050260 Y -2.196548 -1.934662 1.033887 Cl -4.342152 -2.956046 0.179327 O -2.960293 0.046125 -0.061705 C -4.257561 0.451052 -0.578655 C -3.672865 1.153968 0.584799 H -5.045251 -0.309697 -0.437308 H -4.197519 0.924519 -1.574376 H -4.068854 0.870661 1.579446 C -2.992181 2.488897 0.498510 H -3.682648 3.289075 0.836018 H -2.093464 2.493785 1.146886 H -2.676389 2.704790 -0.540780 O -1.345091 -0.388304 4.642902 C -1.861907 -1.015599 5.867050 H -1.286786 -0.478010 6.647333 C -3.352419 -0.754598 6.048610 H -3.670421 -1.118287 7.045614 H -3.558688 0.332959 5.997162 H -3.944799 -1.278854 5.274389 C -1.446364 -2.488337 5.888042 H -0.388804 -2.607290 5.587485 H -2.099102 -3.127144 5.268979 Br -1.560411 -3.217949 7.765063 C -1.729779 -0.831479 3.440732 O -2.560950 -1.801601 3.308366 O -1.216720 -0.261778 2.421630
$\mathbf{I}_{AB}$ (X = Br)	**B** (X = Br)
SCF Done: -4250.16622034 A.U. Si 3.955876 -0.290615 0.102953 Si 0.560633 2.409013 -0.830160 Si -0.145736 -0.434146 -2.072976 Si 3.856785 -1.931380 2.795910 Si 0.180875 2.163577 2.386960 Si 2.289599 -2.254068 -1.719850 Si 1.084712 -0.771058 3.000651 O 2.590185 -1.205307 3.604048 O 0.202496 1.981460 0.719569 O 3.572100 -1.476016 -1.021342 O 1.007227 0.875248 3.067982 O 0.043178 1.187033 -1.854507 O 1.314283 -1.128423 -2.490458 O 4.426464 -0.979155 1.542673 O -0.662403 -1.206724 -0.663739 O 1.343815 -3.032031 -0.583393 O 1.150607 -1.309201 1.409443 H 2.802414 0.634696 0.301303 H 2.038299 2.584529 -1.013314 H 2.808819 -3.237422 -2.697557 H -0.182645 3.640585 -1.234630 H 1.012602 3.368098 2.719283 H 5.152494 0.427101 -0.434921 H 4.979738 -2.066599 3.773941 H -1.217550 2.295149 2.864256 H 3.448339 -3.267759 2.251162 H -1.151311 -0.646951 -3.139416 H 0.070975 -1.460511 3.829614 Si 0.238462 -2.255017 0.398967 O -0.969272 -3.089080 1.051876	SCF Done: -4250.20312292 A.U. Si -1.863586 2.051543 -1.184821 Si -3.195340 -0.786098 1.888058 Si -1.109471 -2.645551 0.466045 Si 1.083482 3.148594 -0.801761 Si -2.086144 1.841715 3.388694 Si -0.862999 -0.851918 -1.964472 Si 0.701277 1.833104 1.891428 O 1.048270 3.114360 0.878701 O -2.513868 0.300007 2.945850 O -1.791804 0.521894 -1.845685 O -0.567427 2.264395 2.863882 O -2.172252 -2.065969 1.603956 O -1.564571 -2.061872 -1.042408 O -0.450083 2.897290 -1.422433 O 0.441042 -2.122567 0.765578 O 0.682742 -0.582738 -1.408053 O 0.234152 0.540666 0.951961 H -2.185209 1.982118 0.273630 H -3.537424 -0.105617 0.598251 H -0.833201 -1.271008 -3.386953 H -4.416581 -1.343397 2.550641 H -3.072306 2.815281 2.810673 H -2.938377 2.776962 -1.931404 H 1.492522 4.528680 -1.193806 H -2.084928 1.899209 4.883051 H 2.011805 2.103232 -1.325398 H -1.164856 -4.124494 0.483490 H 1.879991 1.554891 2.747694 Si 1.136403 -0.687528 0.212013 O 2.703124 -0.561744 0.496017

Y -2.712647 -1.839143 0.579184	Y 3.998890 -0.248136 2.205603
Cl -4.410651 -3.416979 -0.429603	Cl 6.176907 -1.523742 1.926334
O -3.489090 0.080487 -0.363940	O 2.789033 -1.138969 3.633289
C -4.200272 1.213316 0.571749	C 1.745182 -1.798326 4.278180
C -3.026250 1.471413 -0.247008	H 1.995845 -1.959411 5.358250
H -4.104759 0.951027 1.629632	C 0.434997 -1.008134 4.188026
H -5.204555 1.425980 0.181248	H -0.390755 -1.504902 4.735142
H -2.070103 1.546850 0.301747	H 0.587364 0.002910 4.617657
C -3.132670 2.297304 -1.499846	H 0.124913 -0.903210 3.130398
H -3.069381 3.365918 -1.209052	C 1.692728 -3.159828 3.576415
H -2.308984 2.062974 -2.202215	H 2.635587 -3.719295 3.714222
H -4.104566 2.125012 -2.004059	H 1.444262 -3.038579 2.506336
Br -4.191995 3.737081 1.982143	Br 0.235479 -4.423553 4.294220
O -2.367894 0.122947 4.119767	O 4.870837 3.710607 2.742517
C -3.475064 0.121314 5.082779	C 5.207106 4.567888 1.619640
H -3.065899 0.765644 5.886775	H 5.286588 5.562599 2.104347
C -4.733334 0.754610 4.504608	C 6.549871 4.184430 1.002126
H -5.453388 0.957189 5.321854	H 6.825785 4.916845 0.216963
H -4.492640 1.720025 4.006719	H 7.341831 4.184851 1.777060
H -5.217058 0.080318 3.771402	H 6.490628 3.176468 0.546760
C -3.628574 -1.301543 5.623408	C 4.049678 4.621751 0.617770
H -2.648737 -1.738084 5.892020	H 3.067194 4.647195 1.122422
H -4.175660 -1.961988 4.929036	H 4.084140 3.807480 -0.124458
Br -4.695069 -1.301441 7.347275	Br 4.145072 6.347018 -0.461642
C -2.482770 -0.516580 2.948472	C 4.586064 2.400587 2.511424
O -3.441438 -1.341656 2.717934	O 4.446032 1.962772 1.321289
O -1.590437 -0.278967 2.074736	O 4.451750 1.666030 3.536789
I_{BC} (X = Br)	**C** (X = Br)
SCF Done: -4438.66858535 A.U.	SCF Done: -4438.67964864 A.U.
Si -2.537108 1.789380 -1.631582	Si -2.703348 1.778069 -1.985710
Si -5.322768 -1.074997 0.128831	Si -5.652973 -0.942188 -0.368760
Si -2.816789 -2.942430 0.077729	Si -3.139950 -2.783326 0.031310
Si -0.293730 2.757502 0.331918	Si -0.734578 2.937091 0.120000
Si -5.148127 1.560267 1.984082	Si -5.637716 1.839932 1.324667
Si -1.293225 -1.124334 -1.807791	Si -1.358989 -1.089674 -1.745727
Si -2.023888 1.454028 2.416081	Si -2.610103 1.787208 2.177882
O -1.320629 2.759026 1.663883	O -1.900896 3.027193 1.327601
O -5.358413 0.027269 1.370702	O -5.782416 0.294683 0.727654
O -2.105556 0.269448 -2.179395	O -2.108580 0.258693 -2.348421
O -3.642870 1.771750 2.646681	O -4.257568 2.038577 2.223519
O -4.320803 -2.357851 0.489129	O -4.675017 -2.163045 0.203980
O -2.395264 -2.332030 -1.427059	O -2.511659 -2.269808 -1.435666
O -1.251193 2.658535 -1.048850	O -1.548728 2.786171 -1.349877
O -1.663800 -2.494276 1.187377	O -2.139816 -2.273517 1.255870
O -0.309532 -0.902547 -0.481506	O -0.578348 -0.764835 -0.309360
O -1.916657 0.149876 1.378482	O -2.350212 0.378560 1.327918
H -3.585832 1.647997 -0.573645	H -3.846983 1.635452 -1.031843
H -4.884623 -0.421766 -1.144530	H -5.127067 -0.433915 -1.675832
H -0.491779 -1.543282 -2.981687	H -0.395491 -1.590398 -2.753275
H -6.706803 -1.636080 0.006484	H -7.022584 -1.528527 -0.527948
H -5.390477 2.569385 0.900176	H -5.672543 2.818438 0.187826
H -3.076410 2.520556 -2.819659	H -3.158280 2.372572 -3.280362
H 0.415214 4.065016 0.283677	H -0.001004 4.232189 0.070779
H -6.139834 1.727899 3.093451	H -6.792965 2.063326 2.251088
H 0.607591 1.574833 0.353108	H 0.135089 1.745366 0.281914
H -2.907788 -4.422090 0.022367	H -3.244699 -4.262742 0.053949
H -1.424836 1.193056 3.744737	H -2.140565 1.723700 3.580204
Si -0.779741 -1.062142 1.135275	Si -1.227432 -0.859881 1.249650
O 0.459921 -0.988424 2.144328	O -0.098661 -0.796506 2.386844
Y 2.381074 -0.168693 2.608444	Y 1.586706 0.061389 3.357096
Cl 1.849188 2.276322 3.094892	Cl 1.056632 2.551926 3.022226
O 3.340522 0.052629 0.674880	O 2.972497 0.332218 1.443513
C 3.383669 1.017369 -0.351084	C 3.055402 1.130896 0.235250
H 2.924309 1.964244 0.026714	H 2.390053 1.987244 0.470248
C 4.822045 1.303404 -0.785629	C 4.477316 1.617868 -0.013872
H 4.851540 2.064470 -1.592440	H 4.493962 2.283330 -0.900581
H 5.402016 1.680375 0.080660	H 4.837616 2.192701 0.862322
H 5.303442 0.373207 -1.151767	H 5.153138 0.758557 -0.188620
C 2.489621 0.468144 -1.466338	C 2.432703 0.313516 -0.895341
H 1.515600 0.141257 -1.059746	H 1.482308 -0.152275 -0.573893
H 2.972469 -0.349739 -2.033083	H 3.126762 -0.435014 -1.315505

Br 2.007237 1.877300 -2.860320	Br 1.894979 1.511140 -2.441850
C 3.736546 -2.034556 0.444092	C 3.580136 -1.013884 1.557503
O 4.253465 -2.167876 -0.609245	O 4.301667 -1.432039 0.673091
O 3.270725 -2.325504 1.509489	O 3.158823 -1.483567 2.667910
O 4.644569 -1.348443 5.797403	O 2.302895 -0.179083 7.354630
C 6.083632 -1.144653 5.814967	C 3.556024 0.271079 7.940883
H 6.351370 -1.462491 6.843978	H 3.366464 0.132865 9.025421
C 6.797932 -2.034482 4.800223	C 4.733929 -0.599394 7.510079
H 7.895673 -1.932893 4.915610	H 5.645879 -0.296750 8.062754
H 6.523951 -3.095088 4.967837	H 4.522703 -1.662982 7.738281
H 6.515329 -1.746394 3.769525	H 4.918343 -0.493273 6.423830
C 6.395924 0.349398 5.685345	C 3.737038 1.769292 7.678505
H 5.720366 0.956132 6.315702	H 2.791657 2.320294 7.834834
H 6.385028 0.707293 4.642888	H 4.157553 1.989576 6.683560
Br 8.266040 0.743361 6.390544	Br 5.039589 2.569663 9.022801
C 3.936513 -0.971155 4.695859	C 2.128066 -0.078117 6.010464
O 4.507731 -0.361310 3.731738	O 2.999577 0.488044 5.274500
O 2.698910 -1.249056 4.700868	O 1.047949 -0.570108 5.549369
I_{CD} (X = Br)	**D** (X = Br)
SCF Done: -4438.66513602 A.U.	SCF Done: -4438.66478834 A.U.
Si -2.542710 1.480538 -1.593963	Si -0.014388 1.124229 -1.359627
Si -4.639454 -0.524288 1.244543	Si -4.096474 0.311277 -0.064037
Si -2.394415 -2.633089 1.467225	Si -3.565446 -2.700207 -0.472733
Si -0.347360 3.293622 -0.109728	Si 1.541837 0.474684 1.393353
Si -3.047802 1.910506 2.421338	Si -2.078704 1.874815 1.736629
Si -1.218458 -1.383521 -1.005668	Si -1.019894 -1.794385 -1.741394
Si 0.174583 1.657642 2.501049	Si -0.668640 -0.578167 3.041344
O 0.483657 2.436969 1.065117	O 0.918491 -0.755254 2.409016
O -3.706577 0.857978 1.306830	O -2.635042 0.939077 0.464524
O -2.260004 -0.126399 -1.263028	O -0.828327 -0.167781 -2.023919
O -1.465342 1.536247 2.743021	O -1.130269 1.000607 2.801367
O -3.812416 -1.844674 1.847570	O -4.234523 -1.329895 0.210977
O -2.111597 -2.549662 -0.174760	O -2.646434 -2.194726 -1.783758
O -1.737099 2.478500 -0.522492	O 0.402903 0.865673 0.238368
O -1.120916 -1.898544 2.255464	O -2.573827 -3.490816 0.608074
O 0.029644 -0.946579 0.018606	O -0.435306 -2.123280 -0.224631
O 0.777809 0.097461 2.407678	O -1.639113 -1.580799 2.168110
H -4.004727 1.707278 -1.377080	H -0.897938 2.323885 -1.428428
H -5.026228 -0.737160 -0.181252	H -4.179781 0.591965 -1.529555
H -0.729370 -1.996844 -2.257524	H -0.319107 -2.559965 -2.798827
H -5.840198 -0.352269 2.126408	H -5.203719 0.964593 0.705700
H -3.157832 3.297210 1.875278	H -1.264449 3.001490 1.195870
H -2.159835 1.814024 -2.997747	H 1.251827 1.337946 -2.135228
H -0.786069 4.599187 0.487517	H 1.784837 1.690536 2.221308
H -3.803754 1.775162 3.710711	H -3.266183 2.380760 2.502592
H 0.567341 3.489925 -1.268706	H 2.776429 -0.040550 0.750666
H -2.545819 -4.045602 1.893091	H -4.645121 -3.614192 -0.912827
H 0.800395 2.352160 3.642234	H -0.659184 -0.834126 4.493960
Si 0.326537 -1.351638 1.618875	Si -1.127073 -2.824181 1.145734
O 1.626782 -2.254233 1.901030	O -0.059530 -3.768287 1.885019
Y 3.070016 -0.870019 2.826616	Y 1.926060 -3.328892 2.560456
Cl 3.750025 1.548103 3.368304	Cl 2.979127 -5.509410 3.193533
O 3.126684 -0.069568 0.485084	O 2.979532 -2.047433 4.604336
C 2.628562 0.696902 -0.656313	C 3.800328 -0.966379 5.254174
H 1.559258 0.835139 -0.432586	H 4.824540 -1.365387 5.350512
C 3.370062 2.019863 -0.729582	C 3.744372 0.268338 4.381751
H 2.935750 2.635168 -1.541643	H 4.411178 1.023812 4.845642
H 3.264396 2.552067 0.234783	H 4.102991 0.026185 3.361716
H 4.448059 1.856675 -0.934779	H 2.711685 0.671328 4.330950
C 2.798896 -0.209945 -1.861833	C 3.096085 -0.861835 6.622644
H 2.211537 -1.133405 -1.915798	H 3.594643 -1.433463 7.425196
H 3.359723 0.105148 -2.746700	H 2.914516 0.172036 6.957685
Br 0.771052 0.846991 -3.128851	Br 5.785211 0.617747 7.348060
C 4.119226 -0.973840 0.149810	C 1.812104 -2.175746 5.256197
O 4.330575 -1.106189 -1.092560	O 1.755216 -1.497039 6.377241
O 4.636888 -1.540462 1.142785	O 0.917073 -2.867165 4.753784
O 3.334897 -2.747888 6.390241	O 4.367471 -1.914851 -0.352857
C 2.297331 -2.578930 7.398654	C 4.061849 -2.175593 -1.755393
H 2.608313 -3.311480 8.171714	H 4.810505 -1.543173 -2.274700
C 2.300267 -1.172258 7.991424	C 4.270903 -3.639102 -2.130202
H 1.584657 -1.121345 8.836339	H 4.148128 -3.763006 -3.224743

H 3.310493 -0.923294 8.372642 H 2.009069 -0.426468 7.227055 C 0.947074 -3.032005 6.832578 H 1.049392 -3.965216 6.249021 H 0.437467 -2.255244 6.239037 Br -0.328539 -3.495858 8.348228 C 3.231548 -2.066397 5.222439 O 2.209664 -1.341320 4.976984 O 4.186786 -2.203950 4.395006	H 5.295780 -3.958035 -1.855352 H 3.538773 -4.284647 -1.608875 C 2.668276 -1.621830 -2.066527 H 2.532543 -0.623700 -1.611915 H 1.861614 -2.305587 -1.752481 Br 2.431827 -1.324586 -4.051192 C 3.563873 -2.433871 0.604726 O 2.556160 -3.158532 0.298817 O 3.836437 -2.132768 1.806656
Y (X = I)	**Y-PO** (X = I)
SCF Done: -4041.67120400 A.U. Si -3.276473 2.662196 -0.787326 Si -3.026974 -1.672617 0.827194 Si -1.513974 -1.997318 -1.906576 Si -2.496130 2.208796 2.229184 Si -0.347348 -1.260486 2.386319 Si -2.376248 0.671464 -3.107554 Si 0.324556 1.390105 1.151759 O -0.828176 2.026497 2.149251 O -1.894633 -0.940700 1.815987 O -3.249349 1.459966 -1.949710 O 0.698906 -0.177920 1.612436 O -2.234940 -2.379085 -0.477110 O -2.465054 -0.974267 -2.808265 O -3.194203 1.973857 0.731015 O -0.068361 -1.138117 -1.606858 O -0.750978 1.094274 -3.001944 O -0.323843 1.334801 -0.392586 H -4.602176 3.338741 -0.916880 H -3.973466 -0.624858 0.357637 H -2.884705 0.966384 -4.463203 H -3.693346 -2.790555 1.560124 H -0.329933 -0.965009 3.850715 H -2.136852 3.608190 -1.001431 H -3.073523 1.212785 3.173761 H 0.066152 -2.646025 2.046942 H -2.739244 3.614736 2.682802 H -1.173296 -3.234151 -2.640406 H 1.561651 2.201000 1.201721 Si 0.226563 0.585693 -1.765519 O 1.832775 0.527060 -1.922214 Y 2.279373 -1.557399 -1.577312 Cl 2.891536 -2.861245 -3.600334 O 3.017977 -2.444095 2.201389 C 4.049761 -1.728018 2.975090 H 3.792640 -2.047088 4.005006 C 5.449169 -2.211323 2.616467 H 6.183053 -1.771681 3.320798 H 5.507531 -3.314190 2.703188 H 5.722750 -1.911298 1.586751 C 3.812453 -0.221915 2.841747 H 2.732995 0.009673 2.875088 H 4.257292 0.199665 1.923847 I 4.720583 0.906309 4.523786 C 2.891561 -2.243764 0.889663 O 3.672404 -1.450225 0.239944 O 1.932600 -2.847586 0.298490	SCF Done: -4234.68423473 A.U. Si 4.146770 -0.414113 -0.670611 Si 0.608426 2.481335 -0.475470 Si -0.154495 -0.337029 -1.874358 Si 4.714713 -2.054561 1.997889 Si 0.932631 1.951870 2.609146 Si 2.181310 -2.302427 -2.214970 Si 1.958157 -1.084064 2.697887 O 3.529467 -1.494015 3.049669 O 0.219423 2.117072 1.099588 O 3.597734 -1.649894 -1.667607 O 1.833999 0.559343 2.719435 O 0.206805 1.214110 -1.479622 O 1.132870 -1.061223 -2.642168 O 4.877708 -1.032606 0.686939 O -0.434420 -1.268155 -0.487404 O 1.416691 -3.183018 -1.003337 O 1.718349 -1.639513 1.135374 H 3.001020 0.469226 -0.293218 H 2.071832 2.763859 -0.608096 H 2.448997 -3.183572 -3.370255 H -0.223370 3.646572 -0.907075 H 1.915900 3.072394 2.767701 H 5.194746 0.331653 -1.427315 H 6.002517 -2.032173 2.749736 H -0.140897 2.021756 3.637206 H 4.359728 -3.428418 1.519292 H -1.357287 -0.367904 -2.736881 H 1.042339 -1.732197 3.666288 Si 0.595200 -2.465188 0.244769 O -0.532663 -3.256976 1.087842 Y -2.199575 -1.868763 1.024361 Cl -4.360828 -2.835848 0.141941 O -2.886572 0.143130 -0.082558 C -4.170911 0.534134 -0.646294 C -3.679166 1.181991 0.588953 H -4.934033 -0.262362 -0.593678 H -4.074873 1.072893 -1.605227 H -4.117843 0.821254 1.540201 C -3.051298 2.545101 0.625429 H -3.781776 3.287648 1.007425 H -2.165892 2.533423 1.291345 H -2.722137 2.858980 -0.384575 O -1.332979 -0.406433 4.658316 C -1.853962 -1.054145 5.874439 H -1.262546 -0.539089 6.658047 C -3.337528 -0.760078 6.067034 H -3.662830 -1.115356 7.064651 H -3.515601 0.332605 6.018214 H -3.947566 -1.265474 5.294034 C -1.463935 -2.533936 5.844239 H -0.409246 -2.659425 5.536440 H -2.125616 -3.133529 5.195314 I -1.588947 -3.464410 7.856235 C -1.735449 -0.811023 3.449037 O -2.601434 -1.746027 3.295144 O -1.200308 -0.240820 2.440224
I_{AB} (X = I)	**B** (X = I)
SCF Done: -4246.29341210 A.U. Si 4.047341 -0.470490 -0.066963 Si 0.606891 2.491630 -0.633806	SCF Done: -4246.32698757 A.U. Si -1.867092 2.057031 -1.184443 Si -3.201460 -0.794270 1.869347

Si -0.066408 -0.386697 -1.980156	Si -1.111438 -2.646444 0.442994
Si 3.933370 -1.957897 2.727391	Si 1.079960 3.153928 -0.794921
Si 0.216725 2.253060 2.493587	Si -2.095132 1.829122 3.380987
Si 2.228982 -2.392072 -1.762113	Si -0.861421 -0.840679 -1.976879
Si 1.200977 -0.711669 2.939736	Si 0.696798 1.830924 1.894132
O 2.711238 -1.144372 3.524478	O 1.046111 3.114551 0.885111
O -0.099776 2.258387 0.846284	O -2.517262 0.288530 2.928736
O 3.586441 -1.687751 -1.125589	O -1.793856 0.530021 -1.851224
O 1.159149 0.937906 2.914764	O -0.575222 2.258095 2.864326
O 0.355873 1.155309 -1.601284	O -2.179455 -2.074067 1.580040
O 1.283973 -1.219591 -2.501490	O -1.562287 -2.058213 -1.064429
O 4.495796 -1.102171 1.405081	O -0.453210 2.903394 -1.416594
O -0.645386 -1.220144 -0.632100	O 0.436788 -2.122643 0.754413
O 1.302382 -3.107120 -0.568678	O 0.681517 -0.572291 -1.413269
O 1.212442 -1.313479 1.373513	O 0.232746 0.539198 0.952259
H 2.943596 0.522270 0.088202	H -2.190335 1.981678 0.273348
H 2.084580 2.700814 -0.496595	H -3.545045 -0.110087 0.581898
H 2.645058 -3.410088 -2.753072	H -0.826603 -1.250535 -3.401879
H -0.046258 3.647709 -1.318183	H -4.421859 -1.352802 2.532198
H 1.084531 3.441905 2.786949	H -3.081408 2.803167 2.804022
H 5.274028 0.155643 -0.649106	H -2.941145 2.785203 -1.929330
H 5.076382 -2.068481 3.684581	H 1.486693 4.535775 -1.182612
H -1.069099 2.306358 3.230697	H -2.099618 1.879481 4.875586
H 3.466632 -3.310012 2.277590	H 2.009771 2.111852 -1.322415
H -1.105706 -0.381659 -3.033971	H -1.164648 -4.125556 0.454191
H 0.182023 -1.327898 3.818490	H 1.874327 1.552452 2.751800
Si 0.249921 -2.275895 0.424631	Si 1.133684 -0.685995 0.206619
O -0.960157 -3.050437 1.139157	O 2.701192 -0.561435 0.487756
Y -2.687178 -1.788367 0.615637	Y 3.994379 -0.248425 2.197542
Cl -4.380582 -3.380634 -0.370874	Cl 6.167552 -1.535095 1.938809
O -3.411468 0.089658 -0.413787	O 2.775063 -1.131187 3.624147
C -4.394777 1.159909 0.362814	C 1.743416 -1.790258 4.288429
C -3.119875 1.515970 -0.251423	H 2.006960 -1.931116 5.367934
H -4.454563 0.909461 1.428647	C 0.429066 -1.006949 4.193660
H -5.329704 1.245885 -0.206156	H -0.393902 -1.486641 4.760112
H -2.277996 1.694812 0.442592	H 0.584741 0.013246 4.599860
C -3.076277 2.309845 -1.529700	H 0.111265 -0.922205 3.136243
H -3.135897 3.387106 -1.273359	C 1.706941 -3.160129 3.599331
H -2.133507 2.122988 -2.082081	H 2.672835 -3.686165 3.705583
H -3.933231 2.053404 -2.184140	H 1.416514 -3.057754 2.536888
I -5.115035 3.883143 1.633643	I 0.203537 -4.621519 4.449914
O -2.403270 0.214504 4.146963	O 4.857598 3.710979 2.739363
C -3.499560 0.133857 5.122993	C 5.221132 4.573292 1.626021
H -3.114284 0.790792 5.929037	H 5.316871 5.558266 2.127871
C -4.800835 0.702218 4.570676	C 6.564980 4.167628 1.023601
H -5.523769 0.850815 5.396754	H 6.881372 4.909189 0.262980
H -4.626804 1.688187 4.091100	H 7.338712 4.126885 1.815723
H -5.253629 0.020656 3.825383	H 6.488626 3.172724 0.543098
C -3.555087 -1.309067 5.631629	C 4.067613 4.644431 0.619509
H -2.544354 -1.688369 5.871401	H 3.085429 4.699951 1.123701
H -4.066403 -1.984593 4.923639	H 4.081034 3.807434 -0.099248
I -4.684411 -1.487648 7.547027	I 4.191397 6.505216 -0.620019
C -2.492309 -0.418923 2.967156	C 4.580675 2.400048 2.504087
O -3.450477 -1.240075 2.719052	O 4.465252 1.957127 1.313322
O -1.582085 -0.180551 2.114445	O 4.427244 1.668424 3.529272
I_{BC} (X = I)	**C** (X = I)
SCF Done: -4434.79223911 A.U.	SCF Done: -4434.80256906 A.U.
Si -2.101759 2.666581 -1.538731	Si -2.759637 1.778381 -1.954695
Si -5.452943 0.157622 0.063506	Si -5.672852 -0.952264 -0.282594
Si -3.261501 -2.051198 0.049034	Si -3.142132 -2.780933 0.034798
Si 0.087933 3.182184 0.661237	Si -0.742054 2.947707 0.107279
Si -5.051036 2.683114 1.963483	Si -5.607375 1.825775 1.415831
Si -1.419491 -0.419025 -1.723475	Si -1.411018 -1.085046 -1.791971
Si -2.001994 2.097512 2.533008	Si -2.556350 1.758995 2.194122
O -1.066775 3.305511 1.874788	O -1.873362 3.017093 1.348584
O -5.487432 1.187192 1.371470	O -5.787803 0.286127 0.813783
O -1.982184 1.094157 -2.096949	O -2.160375 0.274243 -2.371973
O -3.560924 2.659340 2.691152	O -4.203261 2.000636 2.281471
O -4.677781 -1.269657 0.445212	O -4.670158 -2.163061 0.268881
O -2.713337 -1.441989 -1.414869	O -2.568161 -2.251179 -1.448219
O -0.706099 3.202829 -0.820566	O -1.593441 2.786436 -1.339825

O -2.087346 -1.823664 1.203423	O -2.096274 -2.282521 1.224753
O -0.467421 -0.374667 -0.357355	O -0.581465 -0.764362 -0.381659
O -2.031443 0.826375 1.448951	O -2.305480 0.368564 1.312079
H -3.246486 2.756820 -0.577557	H -3.867262 1.603943 -0.964695
H -4.787951 0.816808 -1.104069	H -5.183199 -0.442299 -1.603091
H -0.650675 -0.944674 -2.876869	H -0.490361 -1.602062 -2.830949
H -6.876284 -0.196963 -0.242426	H -7.041193 -1.549715 -0.406966
H -5.071438 3.685378 0.846424	H -5.657899 2.811392 0.285738
H -2.348102 3.516189 -2.744578	H -3.266082 2.393819 -3.220149
H 0.963725 4.384114 0.714491	H -0.031742 4.255362 0.042749
H -6.047744 3.042406 3.020643	H -6.736618 2.057430 2.371625
H 0.821488 1.890633 0.745640	H 0.158900 1.773633 0.241259
H -3.561316 -3.498908 -0.075147	H -3.245424 -4.260652 0.047054
H -1.525334 1.701402 3.877703	H -2.055371 1.673264 3.584219
Si -1.032005 -0.510439 1.230899	Si -1.184315 -0.868738 1.195461
O 0.146410 -0.606926 2.309703	O -0.025782 -0.810883 2.301768
Y 2.150761 -0.005429 2.779542	Y 1.640497 0.042145 3.305706
Cl 1.922770 2.413620 3.548264	Cl 1.112051 2.535121 2.986990
O 3.047824 0.226260 0.835586	O 3.027416 0.326612 1.396603
C 3.379158 1.206863 -0.116125	C 3.110852 1.138085 0.194755
H 3.046294 2.208791 0.254663	H 2.445289 1.990495 0.443581
C 4.890415 1.251495 -0.355925	C 4.535912 1.625791 -0.039085
H 5.167048 2.043841 -1.080862	H 4.564521 2.314875 -0.907050
H 5.401974 1.456947 0.605891	H 4.893522 2.175005 0.854486
H 5.248606 0.274540 -0.740403	H 5.209457 0.768539 -0.231531
C 2.537917 0.849881 -1.347486	C 2.490333 0.322884 -0.939032
H 1.470819 0.760442 -1.073370	H 1.522360 -0.118329 -0.632888
H 2.890467 -0.075932 -1.838466	H 3.177414 -0.450902 -1.325328
I 2.584969 2.407043 -2.962037	I 1.959783 1.596193 -2.685454
C 3.374173 -1.947420 0.549749	C 3.653576 -1.010411 1.514250
O 3.891365 -2.038723 -0.505395	O 4.385911 -1.420442 0.635096
O 2.888054 -2.228081 1.604392	O 3.232770 -1.484130 2.623542
O 4.393066 -1.720068 5.734011	O 2.251274 -0.216804 7.320426
C 5.847679 -1.693354 5.700409	C 3.475005 0.257726 7.953018
H 6.106182 -2.186304 6.660761	H 3.253154 0.087227 9.026992
C 6.402804 -2.515984 4.538826	C 4.686393 -0.576635 7.541660
H 7.504144 -2.605822 4.623959	H 5.571229 -0.286498 8.142864
H 5.967273 -3.534795 4.562904	H 4.479776 -1.650380 7.721685
H 6.152035 -2.040888 3.571276	H 4.914825 -0.430410 6.468710
C 6.320099 -0.236517 5.756028	C 3.606860 1.765225 7.711387
H 5.758464 0.335304 6.517325	H 2.640542 2.280321 7.863043
H 6.271804 0.268145 4.776162	H 4.023127 2.006741 6.718552
I 8.457736 -0.072564 6.406562	I 4.986482 2.727477 9.189866
C 3.691943 -1.146687 4.714682	C 2.115776 -0.114989 5.971442
O 4.290268 -0.504212 3.790264	O 3.003757 0.457331 5.260337
O 2.431712 -1.287156 4.756327	O 1.051967 -0.612975 5.479989
I_{CD} (X = I)	**D** (X = I)
SCF Done: -4434.78769157 A.U.	SCF Done: -4434.79218857 A.U.
Si -2.444698 1.359447 -0.855565	Si -0.026280 1.116359 -1.364561
Si -4.298132 -0.791015 2.054222	Si -4.103599 0.318905 -0.081953
Si -1.929397 -2.728539 1.890484	Si -3.587722 -2.697663 -0.462675
Si -0.109135 3.107705 0.482549	Si 1.524716 0.465967 1.382835
Si -2.684795 1.588286 3.262174	Si -2.090402 1.872120 1.729383
Si -1.169234 -1.517657 -0.751368	Si -1.024884 -1.809809 -1.706160
Si 0.423227 1.664402 3.105917	Si -0.675093 -0.569192 3.061389
O 0.304607 2.984091 2.099094	O 0.900667 -0.759495 2.404235
O -3.320640 0.562781 2.105176	O -2.639278 0.930408 0.457770
O -2.296216 -0.301660 -0.846387	O -0.820282 -0.191454 -2.022578
O -1.100843 1.221785 3.626342	O -1.139857 1.004268 2.797289
O -3.414000 -2.167303 2.389395	O -4.258720 -1.319323 0.202021
O -1.841438 -2.716239 0.221183	O -2.650941 -2.208761 -1.767593
O -1.362954 2.043585 0.219602	O 0.381975 0.879737 0.239506
O -0.727862 -1.710778 2.451750	O -2.612391 -3.479760 0.639424
O 0.205923 -0.971596 0.034606	O -0.469547 -2.104256 -0.172062
O 1.067925 0.381439 2.229820	O -1.659244 -1.593989 2.229226
H -3.833853 1.673409 -0.402173	H -0.919685 2.307294 -1.451211
H -4.892604 -0.861453 0.686606	H -4.169034 0.591266 -1.549891
H -0.861098 -2.112338 -2.065729	H -0.306035 -2.598037 -2.734148
H -5.353133 -0.692895 3.115224	H -5.211218 0.987907 0.673174
H -2.784300 2.984112 2.736127	H -1.281733 3.003242 1.190003
H -2.197039 1.897360 -2.228666	H 1.242990 1.331428 -2.135084

H	-0.572209	4.514614	0.257018	H	1.789434	1.674220	2.215793
H	-3.471694	1.416379	4.526810	H	-3.283109	2.371243	2.491540
H	1.064089	2.775875	-0.373950	H	2.747276	-0.058039	0.724983
H	-1.773529	-4.110208	2.400962	H	-4.664673	-3.612685	-0.906574
H	1.263369	1.989975	4.270339	H	-0.641992	-0.792921	4.518948
Si	0.630099	-1.161775	1.642228	Si	-1.164723	-2.825114	1.185245
O	1.981384	-1.993657	1.905891	O	-0.097503	-3.789355	1.901077
Y	3.414900	-0.506137	2.657899	Y	1.896444	-3.350815	2.540491
Cl	4.138169	1.939540	2.923792	Cl	2.955048	-5.525358	3.176773
O	3.422809	0.013774	0.235926	O	3.024937	-2.051376	4.635528
C	2.843111	0.587479	-0.981661	C	3.821506	-0.954859	5.276689
H	1.792490	0.786328	-0.706789	H	4.842826	-1.350118	5.418451
C	3.598839	1.856592	-1.337060	C	3.791435	0.252851	4.364986
H	3.103141	2.345673	-2.198714	H	4.453078	1.027737	4.802721
H	3.602997	2.546684	-0.471579	H	4.160781	-0.026622	3.358384
H	4.648072	1.620195	-1.608994	H	2.762647	0.660863	4.284255
C	2.903479	-0.509431	-2.030407	C	3.072302	-0.811792	6.618694
H	2.270901	-1.395183	-1.897078	H	3.538869	-1.370361	7.450399
H	3.415349	-0.367233	-2.986366	H	2.899013	0.232566	6.927013
I	0.700665	0.530332	-3.522455	I	5.986746	0.737109	7.635787
C	4.352747	-0.984376	-0.008724	C	1.832518	-2.145298	5.242213
O	4.460155	-1.337920	-1.220049	O	1.739677	-1.428859	6.340298
O	4.925944	-1.401154	1.027778	O	0.943029	-2.837424	4.732032
O	2.598006	-2.464930	6.006847	O	4.342248	-1.921086	-0.358547
C	1.246141	-2.311559	6.548146	C	4.070940	-2.196021	-1.768008
H	1.143575	-3.241929	7.143321	H	4.841729	-1.574755	-2.268319
C	1.140419	-1.096560	7.466044	C	4.288329	-3.665798	-2.114350
H	0.151318	-1.090481	7.966927	H	4.226652	-3.806260	-3.211996
H	1.926810	-1.138064	8.245764	H	5.294964	-3.985715	-1.779720
H	1.254030	-0.161701	6.884458	H	3.526720	-4.301967	-1.624676
C	0.224203	-2.337773	5.404779	C	2.686086	-1.639066	-2.113684
H	0.502272	-3.067796	4.623415	H	2.548544	-0.631697	-1.678904
H	0.034600	-1.356214	4.943861	H	1.872578	-2.312282	-1.791424
I	-1.788149	-2.999733	6.107669	I	2.426258	-1.343681	-4.298805
C	2.998988	-1.610241	5.039471	C	3.530835	-2.442259	0.589487
O	2.260070	-0.624278	4.700788	O	2.529902	-3.173720	0.278210
O	4.100026	-1.861152	4.453044	O	3.790906	-2.136100	1.794152
Formation of Model A:				Formation of Model B1:			
SCF Done: -4315.84677520 A.U.				SCF Done: -4315.89551182 A.U.			
Si	-5.080151	2.129714	-0.250963	Si	3.695052	-0.375489	-0.683506
Si	-3.133956	-1.485247	0.955118	Si	-0.422459	1.852590	-0.163643
Si	-2.098218	-1.407634	-1.886830	Si	-0.210484	-0.780841	-1.810112
Si	-3.415199	2.690646	2.264685	Si	4.803904	-1.225063	2.200595
Si	-0.150127	-1.474056	1.880976	Si	0.707039	0.748726	2.518577
Si	-3.360785	1.180414	-2.758491	Si	2.217203	-2.495936	-2.347929
Si	-0.428198	1.768166	1.743494	Si	1.920797	-2.076822	2.615279
O	-1.868810	2.141380	2.478448	O	3.309787	-1.260259	2.998375
O	-1.760419	-1.944015	1.764778	O	-0.455110	0.953522	1.300383
O	-4.519036	1.309767	-1.586484	O	3.504806	-1.785708	-1.576016
O	-0.109668	0.190518	1.989895	O	0.639795	-0.950425	2.626732
O	-3.051507	-1.967704	-0.658474	O	-0.059615	0.824677	-1.426681
O	-2.959728	-0.427648	-2.935784	O	1.106511	-1.285042	-2.699499
O	-3.720510	2.814020	0.562417	O	4.642342	-0.625128	0.659735
O	-0.931282	-0.408322	-1.174579	O	-0.112550	-1.626686	-0.326149
O	-1.952023	1.921392	-2.130659	O	1.425604	-3.582382	-1.328193
O	-0.729427	2.057250	0.078179	O	2.075936	-2.569994	1.034383
H	-5.665574	1.118896	0.679904	H	2.356835	0.128835	-0.242531
H	-3.264540	0.007427	0.985369	H	0.727383	2.799193	-0.017762
H	-4.311566	-2.166076	1.557763	H	2.658957	-3.202153	-3.566757
H	0.370952	-2.025288	3.164239	H	-1.725715	2.535870	-0.342936
H	-6.037530	3.203132	-0.616016	H	2.042632	1.213193	2.044851
H	-4.372395	1.660659	2.773162	H	4.409848	0.619995	-1.533378
H	0.605462	-1.936185	0.685206	H	5.664204	-0.291900	2.982205
H	-3.625275	4.021812	2.886204	H	0.258669	1.363884	3.793160
Si	-0.625045	1.198575	-1.361667	H	5.351311	-2.614951	2.143010
O	0.764113	1.533724	-2.193062	H	-1.451570	-1.087287	-2.544915
H	0.662519	2.647224	2.200040	H	1.603151	-3.148323	3.582055
H	-3.743887	1.765439	-4.054153	Si	0.765519	-3.062773	0.102833
H	-1.476685	-2.515259	-2.639441	O	-0.257405	-3.865553	1.040479
Y	-2.025763	4.005818	-0.820064	Y	-1.646755	-1.301452	1.497686
O	-0.285670	4.383686	-1.914865	Cl	-3.122066	-0.149037	-0.187612

C 1.844427 3.450920 -1.337318	Cl -2.492087 -0.666753 3.770318
C 1.038915 4.329302 -2.167442	O -2.552774 -3.294513 1.250662
H 1.547448 3.280835 -0.289924	C -3.695173 -4.068994 1.654133
H 2.892120 3.226976 -1.594731	H -3.858510 -4.858275 0.885588
H 1.286808 4.247596 -3.252755	C -3.446752 -4.701947 3.020535
C 1.774242 5.677531 -1.650722	H -4.315940 -5.312416 3.335602
H 2.844365 5.743842 -1.920995	H -2.554862 -5.359250 2.981786
H 1.205468 6.461702 -2.190554	H -3.271981 -3.911973 3.780502
H 1.622158 5.825572 -0.564463	C -4.870520 -3.090851 1.614893
Cl -1.423791 5.286567 1.275067	H -4.945247 -2.593765 0.630575
Cl -3.997858 4.638405 -2.272363	H -4.800497 -2.333609 2.421061
Br 2.734981 0.652953 -0.118777	Br -6.632927 -4.029261 1.887763
H 1.545268 1.051151 -1.708588	H -1.532329 -3.805832 1.094339
Formation of Model B2:	Formation of Model B3 (leaving HCl):
SCF Done: -4315.87553454 A.U.	SCF Done: -4315.87332079 A.U.
Si -4.200107 2.032521 -1.012583	Si -4.168149 2.042499 -1.018303
Si -2.478203 -1.379839 0.768705	Si -2.459251 -1.406529 0.809205
Si -0.958269 -1.758327 -1.871294	Si -0.941415 -1.785232 -1.844883
Si -2.860268 2.452898 1.843540	Si -2.779370 2.482299 1.820910
Si -0.215032 -1.068328 2.831194	Si -0.165628 -1.085574 2.822100
Si -2.145247 0.794984 -3.198458	Si -2.151530 0.748821 -3.199062
Si 0.175483 1.631484 1.333118	Si 0.233567 1.596255 1.284280
O -1.216913 2.202220 2.005800	O -1.140185 2.197777 1.968420
O -1.741148 -1.473036 2.252743	O -1.723540 -1.448808 2.295882
O -3.248059 1.638540 -2.325460	O -3.239036 1.626535 -2.341582
O 0.438633 0.054334 1.759565	O 0.470138 0.020233 1.721667
O -1.548530 -2.176223 -0.388290	O -1.480647 -2.165832 -0.334441
O -2.064017 -0.787291 -2.665580	O -2.064843 -0.816692 -2.618174
O -3.259890 2.613011 0.232127	O -3.192660 2.597446 0.209696
O 0.415781 -0.735617 -1.663348	O 0.449420 -0.771583 -1.708181
O -0.601869 1.443201 -2.948622	O -0.602388 1.398438 -2.988465
O -0.007504 1.662332 -0.332979	O 0.034818 1.622399 -0.381045
H -4.943222 0.810118 -0.564759	H -4.935593 0.839006 -0.561746
H -2.568606 0.047672 0.324985	H -2.624268 0.010121 0.354323
H -2.464236 0.867050 -4.638626	H -2.488693 0.775516 -4.636703
H -3.813146 -2.030391 0.869791	H -3.759987 -2.124772 0.906775
H -0.398514 -0.470832 4.184946	H -0.295299 -0.482698 4.178735
H -5.113893 3.122267 -1.462560	H -5.060641 3.154129 -1.457650
H -3.592370 1.289239 2.439713	H -3.529892 1.356955 2.464413
H 0.654944 -2.274069 2.809582	H 0.661465 -2.318903 2.768364
H -3.178279 3.733142 2.539923	H -3.058563 3.792502 2.477760
H -0.565620 -2.945293 -2.643000	H -0.589111 -2.986829 -2.613500
H 1.319805 2.488378 1.715403	H 1.395176 2.439034 1.646198
Si 0.401929 0.959741 -1.740606	Si 0.422969 0.922844 -1.795701
O 2.031044 1.118248 -2.057991	O 2.043908 1.089445 -2.165887
Y 2.845686 -1.204612 -2.005154	Y 2.867576 -1.243962 -2.012927
Cl 2.193326 -3.395347 -3.048588	Cl 2.204360 -3.559941 -2.717933
O 3.342541 -1.414474 -0.054742	O 3.412528 -1.226062 -0.069486
C 3.464792 -1.635900 1.322149	C 3.428911 -1.562649 1.291721
H 2.509896 -2.062956 1.711937	H 2.433337 -1.977411 1.577098
C 4.608011 -2.602818 1.630491	C 4.503948 -2.603889 1.602285
H 4.702222 -2.776470 2.721663	H 4.509444 -2.846833 2.684467
H 4.421618 -3.575044 1.132285	H 4.310949 -3.533556 1.030395
H 5.567050 -2.193811 1.249001	H 5.505362 -2.218666 1.316980
C 3.650487 -0.249207 1.949317	C 3.613286 -0.254863 2.078520
H 2.903402 0.454073 1.545169	H 2.965028 0.527703 1.647908
H 4.676021 0.147785 1.821733	H 4.666241 0.090031 2.075224
Br 3.297679 -0.252133 3.950762	Cl 3.107132 -0.441355 3.816929
Cl 4.536358 0.046734 -3.428939	Br 4.645681 -0.124076 -3.738800
H 2.518543 1.655120 -2.716197	H 2.458108 1.671968 -2.833631
Alternative mechanism from model B3:	
Y—CO_2	**Y-CO_2**
SCF Done: -4490.29577797 A.U.	SCF Done: -4490.30116211 A.U.
Si 3.395269 -4.320647 -0.532913	Si -3.266832 2.665005 -0.785334
Si 1.295525 1.386336 0.069825	Si -3.032600 -1.672179 0.822820
Si 0.720242 -0.854176 -1.908854	Si -1.517566 -1.995818 -1.910227
Si 2.753709 -3.986467 2.511925	Si -2.481466 2.206730 2.228767
Si 0.784746 -0.518388 2.330625	Si -0.351140 -1.269794 2.377578
Si 1.073639 -3.755072 -2.501280	Si -2.374365 0.674906 -3.110008
Si -0.286454 -3.360995 2.296674	Si 0.333271 1.377592 1.145234
O 1.184235 -3.634843 3.002397	O -0.814242 2.017318 2.147238

O 0.234512 0.630487 1.205807	O -1.899442 -0.943185 1.812845
O 2.069220 -4.631771 -1.504281	O -3.242828 1.464644 -1.949550
O -0.465954 -1.659522 2.215065	O 0.696799 -0.195540 1.595387
O 1.645844 0.313483 -1.169931	O -2.240791 -2.378107 -0.481952
O 1.608050 -2.158225 -2.462842	O -2.466663 -0.970796 -2.811837
O 2.950232 -3.578377 0.904896	O -3.182984 1.974176 0.731890
O -0.190903 -1.504248 -0.638222	O -0.070830 -1.139452 -1.608626
O -0.512941 -3.804037 -1.931261	O -0.747790 1.093272 -3.007349
O -0.260222 -3.898498 0.725922	O -0.317346 1.336340 -0.398626
H 4.328198 -3.389723 -1.233521	H -4.592151 3.342985 -0.911550
H 2.575830 1.594399 0.816777	H -3.977598 -0.622573 0.354255
H 1.091841 -4.304944 -3.873570	H -2.885140 0.972255 -4.464258
H 0.676293 2.650651 -0.391287	H -3.700887 -2.790280 1.553787
H 2.091484 -1.073488 1.874916	H -0.326933 -0.969359 3.841051
H 4.011135 -5.646614 -0.218167	H -2.126895 3.610511 -0.999761
H 3.649846 -3.129301 3.343416	H -3.062066 1.214441 3.175255
H 0.824307 0.065329 3.699427	H 0.053250 -2.658789 2.041979
H 3.007386 -5.448570 2.707706	H -2.717536 3.614145 2.681930
H -0.076032 -0.311479 -3.027289	H -1.178561 -3.232808 -2.644661
H -1.380522 -3.925419 3.110624	H 1.575922 2.180067 1.201216
Si -0.975604 -3.042088 -0.527557	Si 0.229556 0.583380 -1.771365
O -2.448566 -2.525728 -0.116791	O 1.835301 0.520265 -1.926983
Y -2.044162 -0.439534 0.520309	Y 2.276863 -1.563272 -1.565800
Cl -1.804730 1.335197 -1.282260	Cl 2.904414 -2.875100 -3.579396
O -2.928626 0.099289 2.433795	O 3.013347 -2.428881 2.218580
C -2.653542 -0.125619 3.804435	C 4.045607 -1.717576 2.985717
H -1.546655 -0.163877 3.936347	H 3.810928 -2.036461 4.021070
C -3.205883 0.987317 4.693102	C 5.451438 -2.167690 2.612463
H -2.962889 0.780209 5.755185	H 6.172317 -1.674711 3.294291
H -2.755979 1.959575 4.409465	H 5.553625 -3.264677 2.728271
H -4.305730 1.063694 4.585956	H 5.696866 -1.883384 1.571411
C -3.172434 -1.525819 4.177207	C 3.806177 -0.204113 2.902096
H -2.968807 -2.231198 3.349043	H 2.729700 0.019483 3.018972
H -4.258186 -1.526833 4.394274	H 4.162441 0.216907 1.944952
Cl -2.317915 -2.180991 5.637362	Cl 4.694976 0.627688 4.240189
C -4.795707 0.018904 1.682614	C 2.885138 -2.231794 0.906828
O -4.460362 -0.104338 0.523544	O 3.657609 -1.430385 0.256185
O -5.568639 0.105657 2.570494	O 1.934489 -2.847779 0.314625
Y-CO_2 (closed)	**Y-CO_2 resting state**
SCF Done: -4490.33149382 A.U.	SCF Done: -4108.80112551 A.U.
Si 0.220920 1.269404 -0.524614	Si 4.030943 -0.420785 -0.651281
Si -3.795764 0.111539 -1.001898	Si 0.402450 2.432271 -0.401985
Si -3.037314 -2.931946 -0.920196	Si -0.038741 -0.328039 -1.861523
Si 0.483838 1.146467 2.674437	Si 4.910628 -1.918566 2.008956
Si -3.157368 1.834439 1.558466	Si 0.864309 1.727894 2.570121
Si -0.218655 -1.858928 -0.874002	Si 2.166497 -2.405308 -2.194740
Si -1.958072 -0.422487 3.323235	Si 2.043556 -1.314143 2.789757
O -0.242272 -0.359367 3.127216	O 3.668883 -1.493889 3.058708
O -2.930769 0.882989 0.206764	O 0.055346 1.769971 1.092849
O -0.329399 -0.220966 -1.036166	O 3.543411 -1.744547 -1.568621
O -2.545354 1.071942 2.928880	O 1.663319 0.284681 2.740095
O -3.917149 -1.534585 -0.731448	O 0.445907 1.210021 -1.547965
O -1.562943 -2.542315 -1.607538	O 1.140001 -1.162525 -2.672774
O 0.023592 1.500440 1.125417	O 4.907703 -0.928542 0.662702
O -2.748303 -3.609730 0.596172	O -0.268904 -1.139219 -0.366401
O -0.398199 -2.278604 0.758815	O 1.320386 -3.259655 -1.015377
O -2.571591 -1.521166 2.247884	O 1.792086 -1.962164 1.258915
H -0.644441 2.288628 -1.184904	H 2.822970 0.342187 -0.206081
H -3.079890 0.362538 -2.286837	H 1.746251 3.089444 -0.388561
H 0.997799 -2.443556 -1.469013	H 2.477877 -3.300415 -3.325804
H -5.194392 0.643941 -0.998658	H -0.696845 3.369843 -0.780183
H -2.420188 3.119841 1.396665	H 1.904480 2.806735 2.547326
H 1.660175 1.438478 -0.883051	H 4.935532 0.410841 -1.496206
H -0.091790 2.193371 3.568177	H 6.191355 -1.686624 2.735174
H -4.623678 2.049824 1.778638	H -0.130093 1.909406 3.660289
H 1.947643 1.011171 2.878023	H 4.741704 -3.342336 1.579447
H -3.767538 -3.912442 -1.750968	H -1.322842 -0.354057 -2.596888
H -2.252718 -0.737503 4.737687	H 1.254370 -2.028243 3.818494
Si -1.743155 -2.862480 1.678969	Si 0.599176 -2.537372 0.283393
O -0.897221 -3.542782 2.870465	O -0.658485 -3.225693 1.038801
Y 1.023107 -2.488013 2.686640	Y -2.095567 -1.638393 0.983659

Cl 2.754148 -4.309778 3.018187 O 2.736473 -1.326973 4.219764 C 4.203996 -1.410612 4.323287 H 4.470133 -2.359656 3.808342 C 4.840604 -0.209576 3.666960 H 5.944742 -0.302876 3.713279 H 4.533370 -0.174700 2.602852 H 4.538142 0.732981 4.166612 C 4.347512 -1.546657 5.851296 H 5.152522 -2.237984 6.160530 H 4.468275 -0.567198 6.360824 C 2.189105 -1.953276 5.299328 O 3.075890 -2.121314 6.275110 O 1.022336 -2.306483 5.269960 Cl 2.387579 -1.062930 0.970533	Cl -4.024824 -1.700886 -0.580421 Cl -2.036655 -0.452360 3.166478
Y-CO_2+Cl	**Y-CO_2+Cl--closed**
SCF Done: -4950.58466656 A.U. Si -2.342312 0.924210 -2.434154 Si -4.771692 -1.035442 0.259596 Si -2.438008 -2.847397 1.105582 Si -0.617796 3.047279 -0.790223 Si -3.601679 1.633675 1.324082 Si -1.002023 -1.739020 -1.293927 Si -0.444780 1.766639 2.052169 O 0.038772 2.495319 0.634294 O -3.959364 0.424592 0.219521 O -2.030741 -0.647779 -1.994866 O -2.082404 1.453622 1.945485 O -3.955405 -2.158899 1.190177 O -1.946374 -2.874166 -0.495118 O -1.843131 2.027606 -1.288391 O -1.349849 -1.945117 1.980877 O -0.042507 -1.004595 -0.152480 O 0.292936 0.272805 2.204978 H -3.819723 1.059139 -2.598730 H -4.904932 -1.500103 -1.153621 H -0.206079 -2.438604 -2.329135 H -6.108955 -0.850989 0.911820 H -3.750226 2.950256 0.631146 H -1.638291 1.220219 -3.725866 H -1.242145 4.388900 -0.549432 H -4.574101 1.517292 2.462063 H 0.460535 3.118633 -1.819212 H -2.543295 -4.229453 1.631495 H -0.204783 2.609288 3.235824 Si 0.109704 -1.269107 1.505041 O 1.452976 -1.989403 1.996812 Y 2.715731 -0.360388 2.821462 Cl 2.726906 2.227740 2.966495 O 3.123189 0.066005 0.469581 C 2.602418 0.754961 -0.682575 H 1.565477 0.990109 -0.378221 C 3.365923 2.043905 -0.957218 H 2.908332 2.574055 -1.816815 H 3.313190 2.692405 -0.060455 H 4.425746 1.822390 -1.190610 C 2.522808 -0.229519 -1.851842 H 2.163644 -1.208744 -1.487868 H 3.484247 -0.343849 -2.383111 Cl 1.287262 0.353348 -3.067156 C 4.469423 -0.473490 0.524518 O 5.159369 -0.512488 -0.479684 O 4.658877 -0.844821 1.739363 Cl 3.034087 -1.105300 5.222154	SCF Done: -4950.55307075 A.U. Si -2.484160 1.535569 -1.606572 Si -4.597722 -0.553063 1.177197 Si -2.314777 -2.643861 1.385718 Si -0.300998 3.264710 -0.050362 Si -3.049906 1.867725 2.421465 Si -1.135403 -1.267876 -1.032923 Si 0.167562 1.612875 2.555372 O 0.505556 2.363446 1.110286 O -3.737038 0.874120 1.272368 O -2.269359 -0.083346 -1.273085 O -1.477293 1.438097 2.726764 O -3.721620 -1.839555 1.781672 O -1.996829 -2.496514 -0.240021 O -1.721256 2.518004 -0.486017 O -1.038700 -1.984736 2.240201 O 0.037512 -0.809176 0.072815 O 0.804347 0.056731 2.529079 H -3.950333 1.787718 -1.445963 H -4.961480 -0.764544 -0.254430 H -0.606799 -1.892818 -2.261130 H -5.816735 -0.445891 2.045637 H -3.127979 3.276027 1.927844 H -2.049894 1.884378 -2.992091 H -0.695931 4.568778 0.580795 H -3.807255 1.705999 3.707757 H 0.619160 3.470116 -1.202624 H -2.504687 -4.069076 1.751514 H 0.714639 2.353195 3.708390 Si 0.371652 -1.336620 1.623855 O 1.720719 -2.194940 1.804082 Y 3.146814 -0.862207 2.809964 Cl 3.628143 1.573638 3.449050 O 3.271948 0.095864 0.496874 C 2.636589 0.742940 -0.653308 H 1.609684 0.944140 -0.317121 C 3.388401 2.018030 -0.986574 H 2.869857 2.516916 -1.828213 H 3.394114 2.686788 -0.104558 H 4.434933 1.796300 -1.281525 C 2.622378 -0.303295 -1.752301 H 1.969864 -1.174711 -1.632131 H 3.036518 -0.099628 -2.744368 Cl 0.593303 0.764367 -2.706199 C 4.111805 -0.930400 0.137249 O 4.153614 -1.188539 -1.106405 O 4.679627 -1.485385 1.112241 Cl 3.773676 -2.161702 4.873113
Y-CO_2+Cl-closed	Formation of Model B3 (leaving HBr):
SCF Done: -4950.53854772 A.U. Si 0.061417 1.242712 -1.040475 Si -4.041090 0.256849 -0.464314 Si -3.366102 -2.757167 -0.795413 Si 1.252343 0.561711 1.842460 Si -2.457898 1.778333 1.774269	SCF Done: -4315.89348264 A.U. Si 3.690317 -0.370637 -0.693011 Si -0.424537 1.853020 -0.159008 Si -0.222061 -0.793795 -1.792751 Si 4.811005 -1.207098 2.192767 Si 0.732454 0.759771 2.513142

Si	-0.658608	-1.739198	-1.497467	Si	2.208535	-2.501011	-2.341969
Si	-1.087032	-0.606588	3.265290	Si	1.933029	-2.067499	2.622337
O	0.532712	-0.709405	2.733644	O	3.321053	-1.245909	2.998725
O	-2.744992	0.858631	0.404307	O	-0.448144	0.961892	1.310439
O	-0.546200	-0.109729	-1.805710	O	3.498402	-1.783198	-1.581428
O	-1.630437	0.934545	2.953016	O	0.651508	-0.939560	2.629023
O	-4.199156	-1.395743	-0.301389	O	-0.076669	0.813590	-1.416683
O	-2.198580	-2.278034	-1.900115	O	1.089468	-1.295812	-2.689640
O	0.228173	1.046423	0.609103	O	4.638748	-0.614582	0.650118
O	-2.629381	-3.486214	0.510247	O	-0.115768	-1.635051	-0.305808
O	-0.466043	-1.962135	0.130361	O	1.426989	-3.586030	-1.314331
O	-1.961815	-1.692509	2.376624	O	2.085439	-2.564496	1.042284
H	-0.883475	2.374159	-1.276758	H	2.352136	0.134205	-0.252728
H	-3.808913	0.608802	-1.898750	H	0.729443	2.796658	-0.029241
H	0.335425	-2.469127	-2.319610	H	2.644223	-3.208287	-3.562335
H	-5.306225	0.859952	0.067325	H	-1.727757	2.537750	-0.332503
H	-1.667358	2.987823	1.403569	H	2.062820	1.209455	2.011656
H	1.414430	1.536312	-1.619799	H	4.403447	0.622122	-1.547432
H	1.375717	1.728648	2.768868	H	5.670468	-0.266173	2.965856
H	-3.788897	2.168703	2.351635	H	0.308752	1.387190	3.790014
H	2.543077	0.072165	1.302241	H	5.364340	-2.594640	2.138039
H	-4.312299	-3.709037	-1.423022	H	-1.469957	-1.105605	-2.514414
H	-1.171036	-0.838683	4.720521	H	1.616534	-3.134061	3.594464
Si	-1.312079	-2.817285	1.305820	Si	0.772494	-3.069917	0.120752
O	-0.306500	-3.821616	2.065489	O	-0.239297	-3.880298	1.061085
Y	1.614604	-3.329965	2.832982	Y	-1.632848	-1.290190	1.519277
Cl	2.590507	-5.479584	3.670182	Cl	-3.136613	-0.138332	-0.134472
O	2.914131	-1.917157	4.502515	Br	-2.525964	-0.627378	3.959956
C	4.009832	-0.999058	5.046081	O	-2.528353	-3.282186	1.303821
H	4.928873	-1.606896	5.080067	C	-3.688029	-4.058977	1.649428
C	4.132431	0.180715	4.108168	H	-3.830220	-4.828921	0.857202
H	4.984164	0.777158	4.497489	C	-3.497068	-4.726750	3.007407
H	4.338402	-0.162899	3.075389	H	-4.401307	-5.307712	3.276254
H	3.209533	0.798453	4.119262	H	-2.628456	-5.415184	2.985082
C	3.489065	-0.704884	6.461017	H	-3.322226	-3.957993	3.789046
H	3.983594	-1.282253	7.256880	C	-4.874492	-3.089562	1.597023
H	3.436240	0.360772	6.727097	H	-4.910704	-2.573879	0.618578
Cl	6.103490	0.135056	6.697543	H	-4.800252	-2.331607	2.404211
C	1.852712	-1.915092	5.333246	Cl	-6.442826	-3.962313	1.812165
O	2.013440	-1.203726	6.409497	H	-1.518130	-3.801676	1.136968
O	0.848191	-2.568971	4.999616				
Cl	3.030558	-2.586110	0.869180				
Y-CO_2+Br				**Y-CO_2+Br--closed**			
SCF Done: -4503.89185251 A.U.				SCF Done: -4503.85928781 A.U.			
Si	-2.349503	0.922212	-2.435291	Si	-2.491292	1.538960	-1.601889
Si	-4.772947	-1.042993	0.260739	Si	-4.596494	-0.557668	1.183106
Si	-2.432770	-2.849904	1.104050	Si	-2.309850	-2.645957	1.382186
Si	-0.624838	3.046895	-0.793791	Si	-0.305918	3.267588	-0.048260
Si	-3.606426	1.626605	1.325653	Si	-3.047345	1.860767	2.428999
Si	-1.004786	-1.739328	-1.300450	Si	-1.139097	-1.263494	-1.039070
Si	-0.452102	1.767679	2.050847	Si	0.169458	1.613774	2.555385
O	0.028870	2.503730	0.636034	O	0.505322	2.370168	1.113123
O	-3.964726	0.419639	0.219360	O	-3.735673	0.869710	1.278720
O	-2.038008	-0.650844	-1.998728	O	-2.276253	-0.081620	-1.275613
O	-2.086030	1.442164	1.945673	O	-1.473022	1.430108	2.729124
O	-3.950376	-2.163395	1.189616	O	-3.716655	-1.844442	1.781762
O	-1.941887	-2.876577	-0.497050	O	-1.993612	-2.495171	-0.243606
O	-1.847894	2.022630	-1.287468	O	-1.724801	2.515645	-0.478507
O	-1.343936	-1.943412	1.975897	O	-1.032707	-1.983693	2.234912
O	-0.044309	-0.999379	-0.162037	O	0.034541	-0.801154	0.065666
O	0.299317	0.278058	2.194136	O	0.814208	0.059121	2.519388
H	-3.826793	1.058099	-2.598355	H	-3.956839	1.790934	-1.436922
H	-4.906653	-1.507878	-1.152271	H	-4.963656	-0.766204	-0.248002
H	-0.208240	-2.436926	-2.336310	H	-0.610726	-1.887276	-2.267775
H	-6.109094	-0.862598	0.915860	H	-5.812462	-0.453230	2.055757
H	-3.751327	2.944587	0.634878	H	-3.125067	3.270257	1.939063
H	-1.645096	1.219982	-3.726339	H	-2.058799	1.893150	-2.986509
H	-1.249401	4.389719	-0.561877	H	-0.701805	4.571707	0.581805
H	-4.577499	1.509738	2.464279	H	-3.800689	1.695316	3.716816
H	0.456506	3.111565	-1.820094	H	0.612075	3.471958	-1.202321
H	-2.532856	-4.231042	1.632309	H	-2.494086	-4.071751	1.747131

H -0.210260 2.606156 3.237047 Si 0.109983 -1.263702 1.494475 O 1.460245 -1.978841 1.979537 Y 2.713093 -0.351812 2.801941 Cl 2.731479 2.225725 2.984883 O 3.135272 0.087950 0.468209 C 2.609342 0.767818 -0.687956 H 1.574538 1.008562 -0.380128 C 3.375531 2.051293 -0.979771 H 2.915375 2.572820 -1.843212 H 3.329754 2.711585 -0.091377 H 4.433438 1.823893 -1.215926 C 2.521540 -0.227584 -1.847490 H 2.157341 -1.201299 -1.474013 H 3.481455 -0.351905 -2.379408 Cl 1.287157 0.350888 -3.065015 C 4.479920 -0.460953 0.523899 O 5.170897 -0.502339 -0.478321 O 4.661697 -0.834820 1.739503 Br 3.005968 -1.166742 5.387678	H 0.720674 2.348777 3.709898 Si 0.371847 -1.332140 1.613672 O 1.726543 -2.186647 1.783828 Y 3.144999 -0.855399 2.787304 Cl 3.644118 1.559564 3.463138 O 3.284536 0.109923 0.487693 C 2.638361 0.751013 -0.661988 H 1.612173 0.948038 -0.320833 C 3.382934 2.027788 -1.004041 H 2.857449 2.519622 -1.845485 H 3.389737 2.701815 -0.126097 H 4.429002 1.809865 -1.303373 C 2.623816 -0.300061 -1.756728 H 1.967214 -1.168241 -1.634709 H 3.031531 -0.096548 -2.751541 Cl 0.586596 0.770419 -2.705183 C 4.117015 -0.922330 0.126274 O 4.151204 -1.183101 -1.116825 O 4.683468 -1.479680 1.100932 Br 3.764286 -2.261597 5.012976
Y-CO_2+Br-closed	**Y-CO_2 resting state (X = Br)**
SCF Done: -4503.89185251 A.U. Si -2.349503 0.922212 -2.435291 Si -4.772947 -1.042993 0.260739 Si -2.432770 -2.849904 1.104050 Si -0.624838 3.046895 -0.793791 Si -3.606426 1.626605 1.325653 Si -1.004786 -1.739328 -1.300450 Si -0.452102 1.767679 2.050847 O 0.028870 2.503730 0.636034 O -3.964726 0.419639 0.219360 O -2.038008 -0.650844 -1.998728 O -2.086030 1.442164 1.945673 O -3.950376 -2.163395 1.189616 O -1.941887 -2.876577 -0.497050 O -1.847894 2.022630 -1.287468 O -1.343936 -1.943412 1.975897 O -0.044309 -0.999379 -0.162037 O 0.299317 0.278058 2.194136 H -3.826793 1.058099 -2.598355 H -4.906653 -1.507878 -1.152271 H -0.208240 -2.436926 -2.336310 H -6.109094 -0.862598 0.915860 H -3.751327 2.944587 0.634878 H -1.645096 1.219982 -3.726339 H -1.249401 4.389719 -0.561877 H -4.577499 1.509738 2.464279 H 0.456506 3.111565 -1.820094 H -2.532856 -4.231042 1.632309 H -0.210260 2.606156 3.237047 Si 0.109983 -1.263702 1.494475 O 1.460245 -1.978841 1.979537 Y 2.713093 -0.351812 2.801941 Cl 2.731479 2.225725 2.984883 O 3.135272 0.087950 0.468209 C 2.609342 0.767818 -0.687956 H 1.574538 1.008562 -0.380128 C 3.375531 2.051293 -0.979771 H 2.915375 2.572820 -1.843212 H 3.329754 2.711585 -0.091377 H 4.433438 1.823893 -1.215926 C 2.521540 -0.227584 -1.847490 H 2.157341 -1.201299 -1.474013 H 3.481455 -0.351905 -2.379408 Cl 1.287157 0.350888 -3.065015 C 4.479920 -0.460953 0.523899 O 5.170897 -0.502339 -0.478321 O 4.661697 -0.834820 1.739503 Br 3.005968 -1.166742 5.387678	SCF Done: -3662.10567469 A.U. Si 3.955285 -0.312045 -0.581768 Si 0.481340 2.410275 -0.436108 Si -0.129393 -0.369388 -1.876789 Si 4.863876 -1.912190 2.005737 Si 1.056247 1.763298 2.574925 Si 2.185580 -2.344412 -2.170189 Si 2.003895 -1.348142 2.837509 O 3.619747 -1.617457 3.094400 O 0.278708 1.772786 1.087869 O 3.532746 -1.634929 -1.531110 O 1.695337 0.264144 2.879981 O 0.236724 1.196359 -1.564322 O 1.116891 -1.140842 -2.651382 O 4.812246 -0.810932 0.748052 O -0.355412 -1.203306 -0.390366 O 1.362790 -3.234074 -1.000362 O 1.721755 -1.899267 1.273338 H 2.710946 0.400647 -0.154947 H 1.869468 2.942077 -0.612185 H 2.542662 -3.224228 -3.299690 H -0.560374 3.451232 -0.683222 H 2.196626 2.734515 2.506903 H 4.849086 0.565847 -1.390254 H 6.145696 -1.702000 2.736527 H 0.068249 2.110984 3.632141 H 4.733327 -3.298537 1.456715 H -1.388232 -0.470318 -2.646880 H 1.187218 -2.082540 3.829133 Si 0.583452 -2.545222 0.282648 O -0.649690 -3.308609 1.011813 Y -2.172478 -1.814853 0.909070 Cl -4.088697 -1.982521 -0.657337 Br -2.109439 -0.346822 3.120500
Alternative mechanism from model B2:	
Y-CO_2+Cl	**Y-CO_2+Cl--closed**

SCF Done: -4503.89250840 A.U.			
Si	-2.380746	0.922776	-2.430402
Si	-4.790298	-1.033204	0.296316
Si	-2.455509	-2.842916	1.120013
Si	-0.628245	3.052510	-0.797291
Si	-3.599984	1.639680	1.327413
Si	-1.032825	-1.750130	-1.298887
Si	-0.436274	1.770355	2.036722
O	0.047595	2.492427	0.615503
O	-3.961956	0.417347	0.238893
O	-2.043950	-0.648786	-2.008328
O	-2.075608	1.466875	1.936991
O	-3.973283	-2.158337	1.224686
O	-1.986855	-2.866847	-0.487576
O	-1.841024	2.020736	-1.298751
O	-1.355897	-1.936945	1.976152
O	-0.053971	-1.015271	-0.172114
O	0.294456	0.272018	2.183687
H	-3.863199	1.055214	-2.543816
H	-4.942321	-1.504761	-1.112757
H	-0.248549	-2.465792	-2.331909
H	-6.118325	-0.831807	0.961852
H	-3.754487	2.947886	0.620161
H	-1.724070	1.225039	-3.744972
H	-1.272145	4.381599	-0.538159
H	-4.563983	1.535189	2.473550
H	0.446275	3.152168	-1.828267
H	-2.549668	-4.224935	1.647896
H	-0.188153	2.610864	3.219953
Si	0.103864	-1.271428	1.487206
O	1.445501	-1.993950	1.979951
Y	2.695961	-0.362884	2.821015
Cl	2.727544	2.226003	2.949182
O	3.128579	0.040164	0.460556
C	2.629208	0.735102	-0.701268
H	1.576601	0.939818	-0.427509
C	3.371551	2.045580	-0.926692
H	2.910221	2.605095	-1.765201
H	3.301155	2.654870	-0.003964
H	4.436906	1.853098	-1.160214
C	2.637860	-0.255324	-1.861943
H	2.229191	-1.229228	-1.539171
H	3.626187	-0.366701	-2.339326
Br	1.367340	0.370690	-3.328541
C	4.492007	-0.456332	0.552764
O	5.211825	-0.469127	-0.430551
O	4.658768	-0.825232	1.771003
Cl	2.963689	-1.097447	5.229968

SCF Done: -4503.87294824 A.U.			
Si	-2.530868	1.505596	-1.570035
Si	-4.620419	-0.545317	1.254877
Si	-2.378656	-2.647392	1.463656
Si	-0.302490	3.249255	-0.065818
Si	-3.023152	1.881369	2.431891
Si	-1.200440	-1.342958	-0.989363
Si	0.205043	1.642149	2.552593
O	0.530676	2.381993	1.100157
O	-3.662744	0.820097	1.312932
O	-2.260822	-0.116774	-1.307413
O	-1.440292	1.525009	2.766064
O	-3.807270	-1.879464	1.848047
O	-2.084779	-2.525386	-0.173846
O	-1.707434	2.451732	-0.464070
O	-1.116629	-1.916743	2.274687
O	-0.005262	-0.847131	0.074463
O	0.791478	0.066827	2.510626
H	-3.989811	1.737603	-1.338900
H	-5.019620	-0.749303	-0.168792
H	-0.647376	-1.959753	-2.212282
H	-5.812192	-0.358006	2.145770
H	-3.146947	3.267896	1.888829
H	-2.145737	1.891227	-2.959525
H	-0.715030	4.561873	0.534306
H	-3.789436	1.734257	3.714265
H	0.598884	3.425251	-1.238128
H	-2.519823	-4.069413	1.859103
H	0.796413	2.361987	3.695568
Si	0.319746	-1.335923	1.645862
O	1.628469	-2.243171	1.867032
Y	3.107739	-0.895802	2.776034
Cl	3.663330	1.566272	3.248305
O	3.101549	-0.066383	0.413179
C	2.614573	0.696638	-0.737103
H	1.540558	0.821287	-0.528905
C	3.349270	2.023764	-0.794149
H	2.924289	2.640082	-1.610191
H	3.226310	2.548008	0.172670
H	4.431206	1.867372	-0.983711
C	2.819032	-0.213646	-1.934868
H	2.228483	-1.134248	-2.007391
H	3.374755	0.114708	-2.818492
Br	0.771662	0.846538	-3.220884
C	4.100446	-0.951365	0.088729
O	4.325959	-1.091400	-1.151326
O	4.626993	-1.510715	1.086651
Cl	3.746627	-2.099910	4.892277

Y-CO_2+Cl-closed

SCF Done: -4503.87305401 A.U.			
Si	0.079383	1.192348	-1.078752
Si	-4.033255	0.278876	-0.478993
Si	-3.413995	-2.751130	-0.797482
Si	1.252503	0.540661	1.824355
Si	-2.425315	1.789647	1.751537
Si	-0.694460	-1.777916	-1.516829
Si	-1.088866	-0.612232	3.242693
O	0.534006	-0.742307	2.710213
O	-2.729304	0.866454	0.388907
O	-0.566584	-0.150487	-1.828870
O	-1.600647	0.936855	2.929412
O	-4.213951	-1.370434	-0.304280
O	-2.241318	-2.303101	-1.909580
O	0.245911	1.002046	0.572881
O	-2.683875	-3.486318	0.510894
O	-0.500334	-1.994790	0.112909
O	-1.984008	-1.684692	2.360695
H	-0.839692	2.343927	-1.317692
H	-3.791789	0.617550	-1.914723
H	0.289960	-2.522928	-2.336289
H	-5.289356	0.903598	0.048053

H	-1.615060	2.983678	1.374604
H	1.438043	1.447391	-1.661235
H	1.342769	1.708291	2.752438
H	-3.745824	2.199541	2.337544
H	2.561474	0.064956	1.316950
H	-4.381081	-3.688989	-1.413029
H	-1.163380	-0.846764	4.698743
Si	-1.357264	-2.827473	1.294492
O	-0.355222	-3.828895	2.066546
Y	1.576052	-3.304530	2.773963
Cl	2.590912	-5.418288	3.646779
O	2.954224	-1.897791	4.490580
C	4.007769	-0.971311	5.045064
H	4.961761	-1.524418	4.998665
C	4.031148	0.286439	4.207158
H	4.848408	0.922129	4.606971
H	4.238921	0.042291	3.147125
H	3.069203	0.835303	4.284629
C	3.515050	-0.809353	6.498431
H	4.056223	-1.441297	7.223910
H	3.495628	0.233646	6.853396
Br	6.444388	0.283074	6.845857
C	1.903917	-1.948992	5.332327
O	2.092181	-1.293074	6.450311
O	0.891621	-2.575205	4.994399
Cl	2.972071	-2.587130	0.792502

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