Supporting Information

Tetrachlorocatecholates of tertiary arsines as a novel class of Lewis acids

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1. NMR spectra

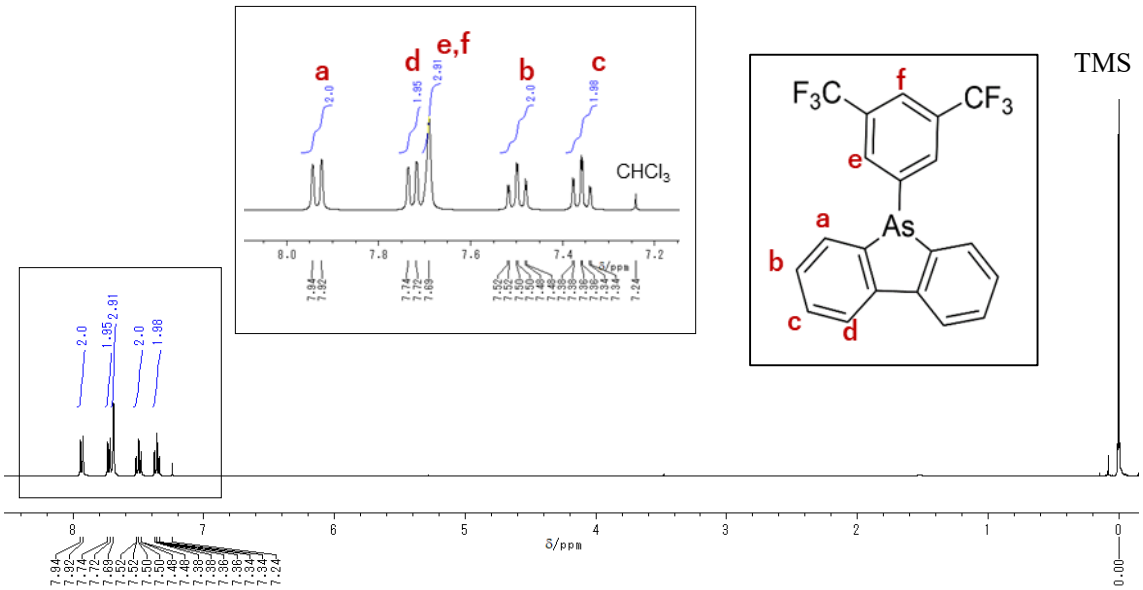


Figure S1. ^{1}H-NMR (400 MHz) spectrum for **5'** in $CDCl_3$.

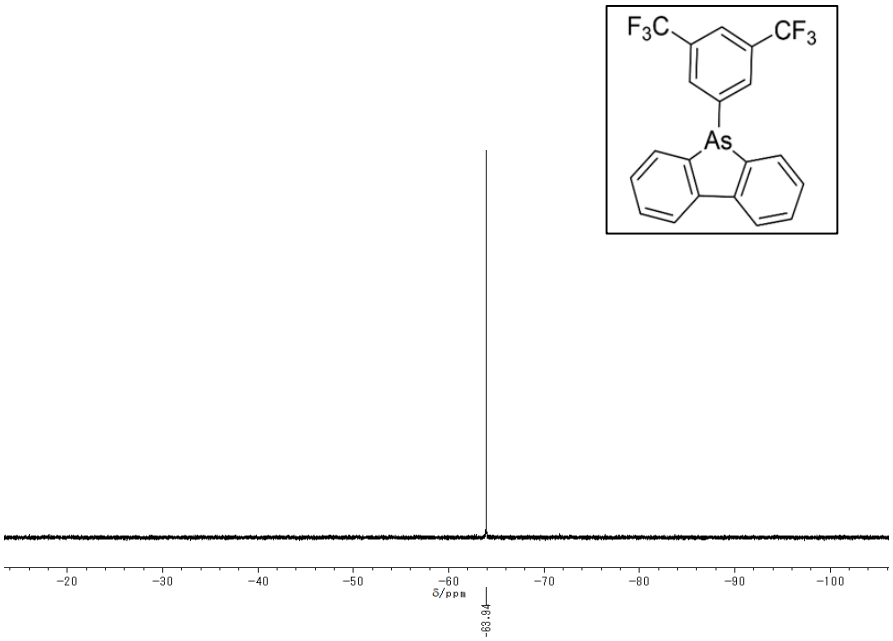


Figure S2. ^{19}F-NMR (376 MHz) spectrum for **5'** in $CDCl_3$.

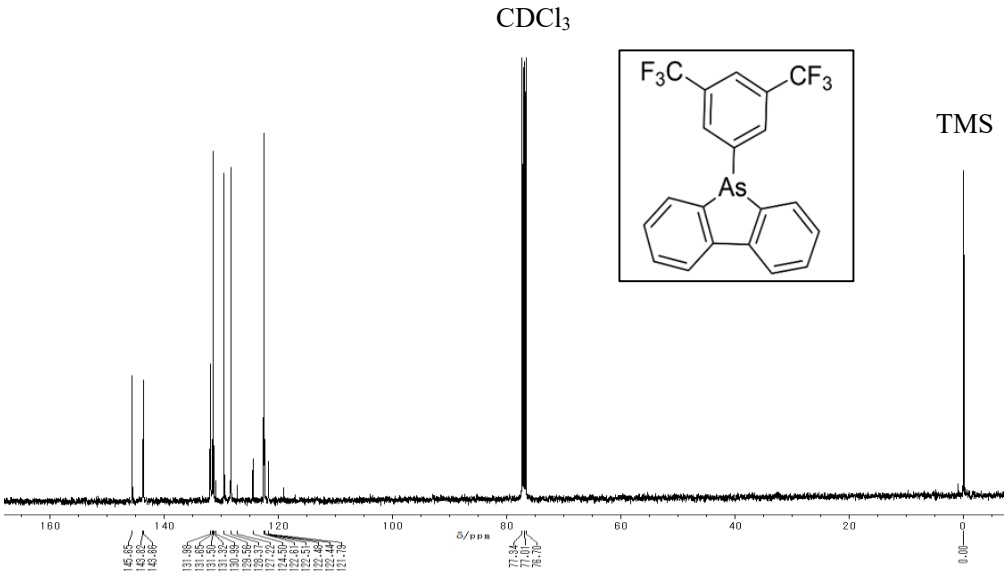


Figure S3. ^{13}C-NMR (100 MHz) spectrum for **5'** in $CDCl_3$.

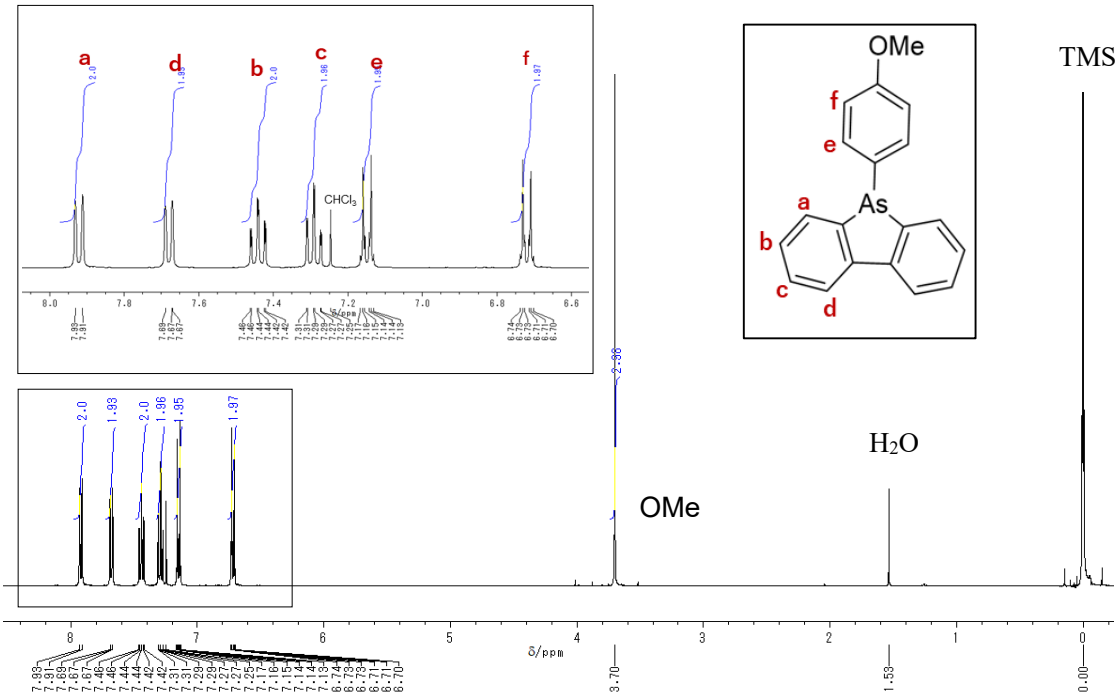


Figure S4. ^{1}H-NMR (400 MHz) spectrum for **7'** in $CDCl_3$.

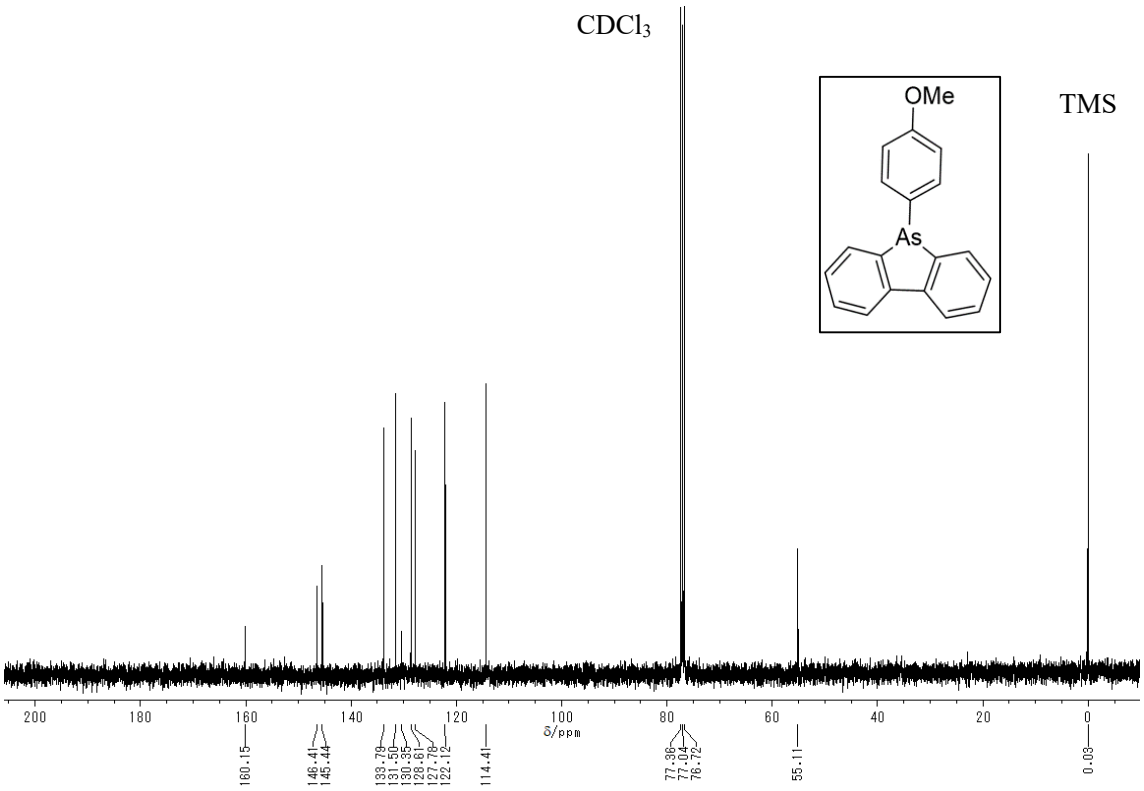


Figure S5. ^{13}C-NMR (100 MHz) spectrum for **7'** in $CDCl_3$.

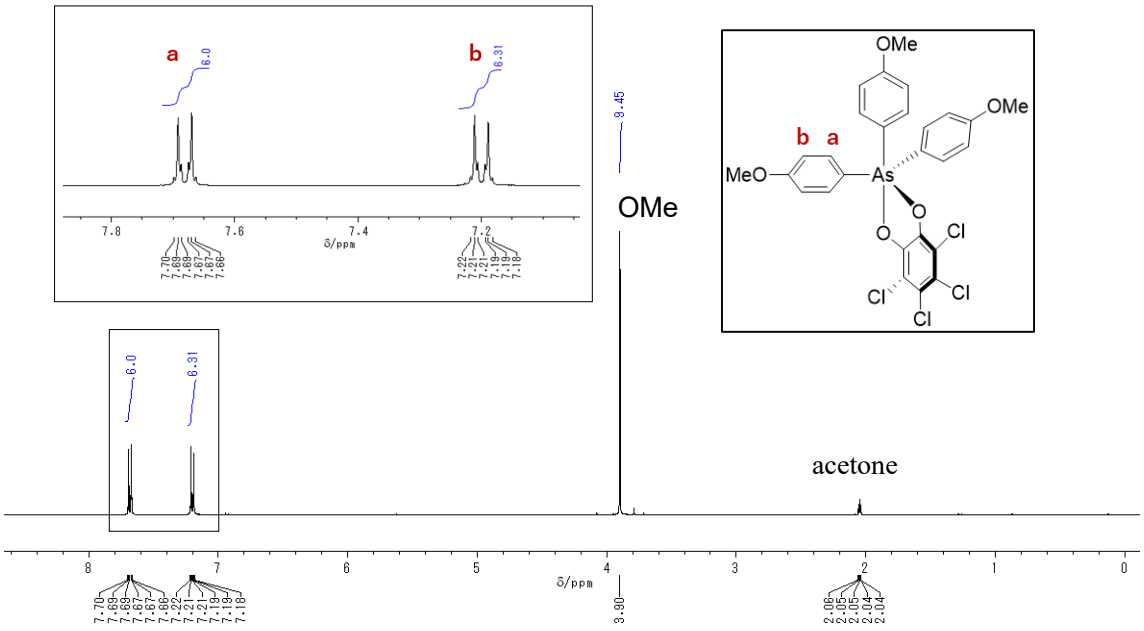


Figure S6. ^{1}H-NMR (400 MHz) spectrum for **3** in acetone-d_6.

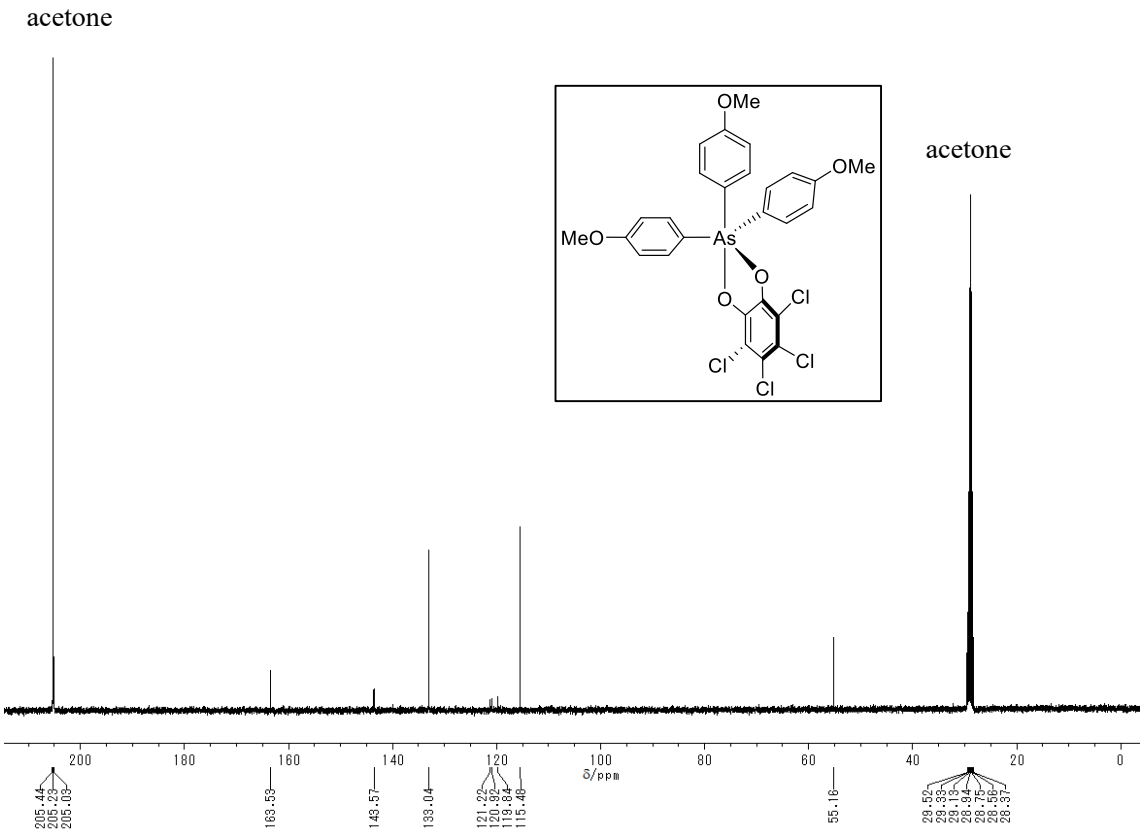


Figure S7. ^{13}C-NMR (100 MHz) spectrum for **3** in acetone-d_6.

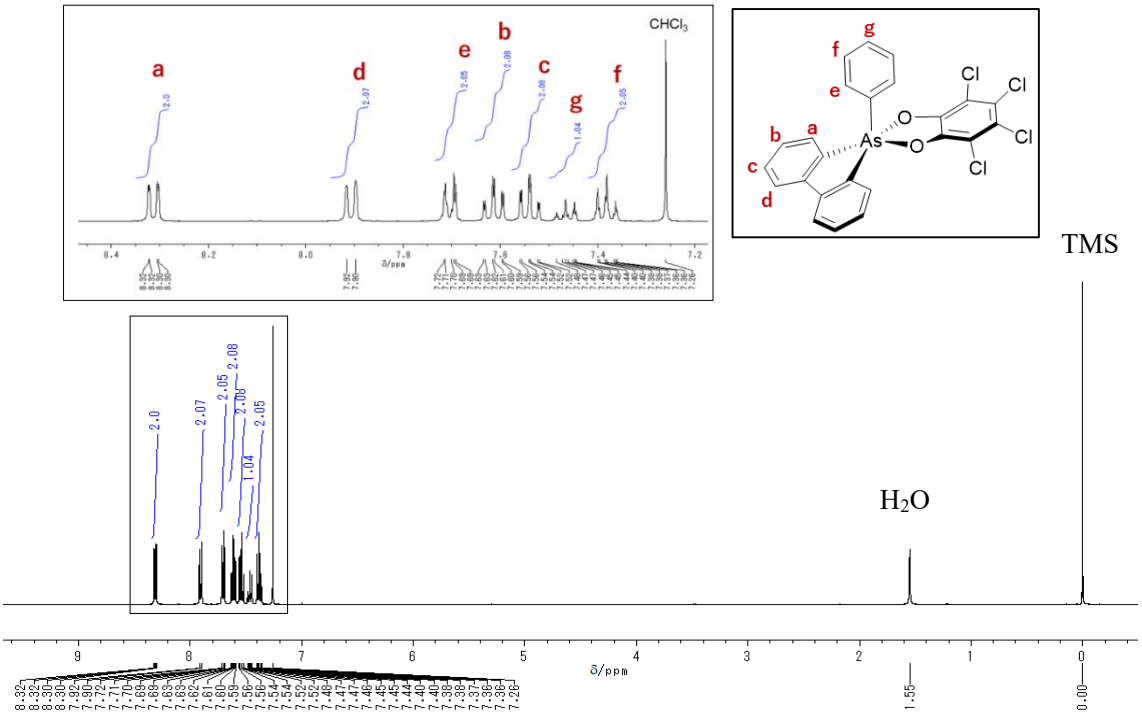


Figure S8. ^{1}H-NMR (400 MHz) spectrum for **4** in $CDCl_3$.

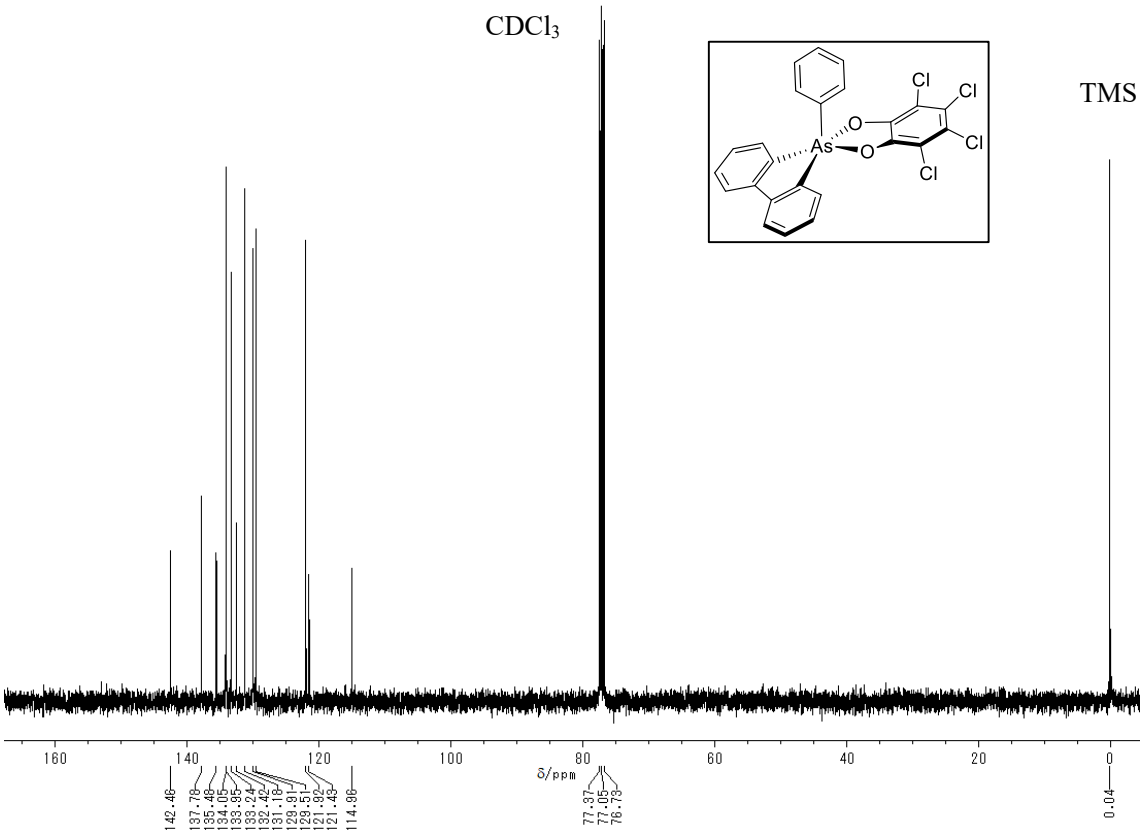


Figure S9. ^{13}C-NMR (100 MHz) spectrum for **4** in $CDCl_3$.

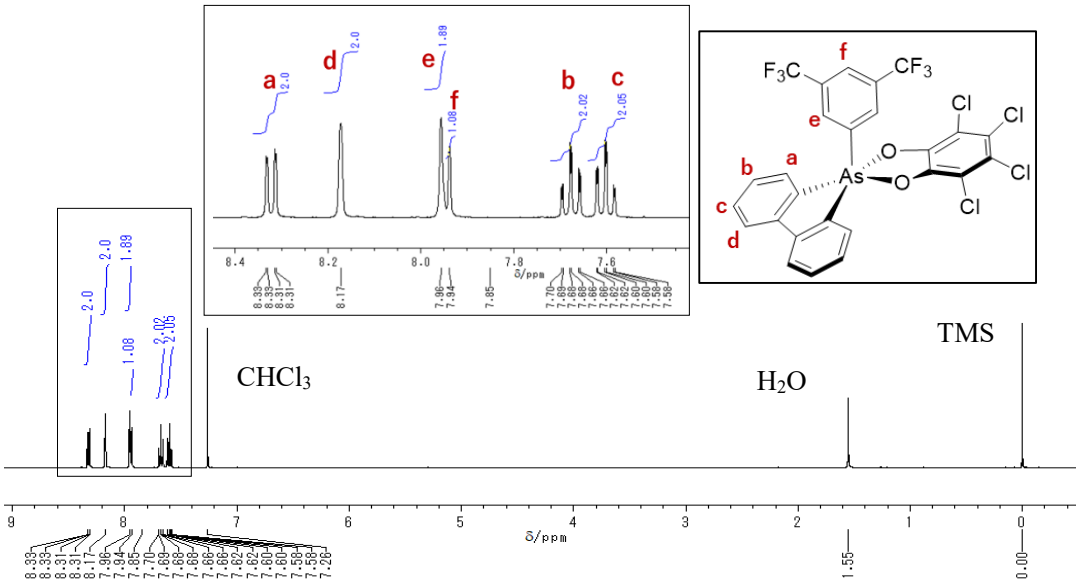


Figure S10. ^{1}H-NMR (400 MHz) spectrum for **5** in $CDCl_3$.

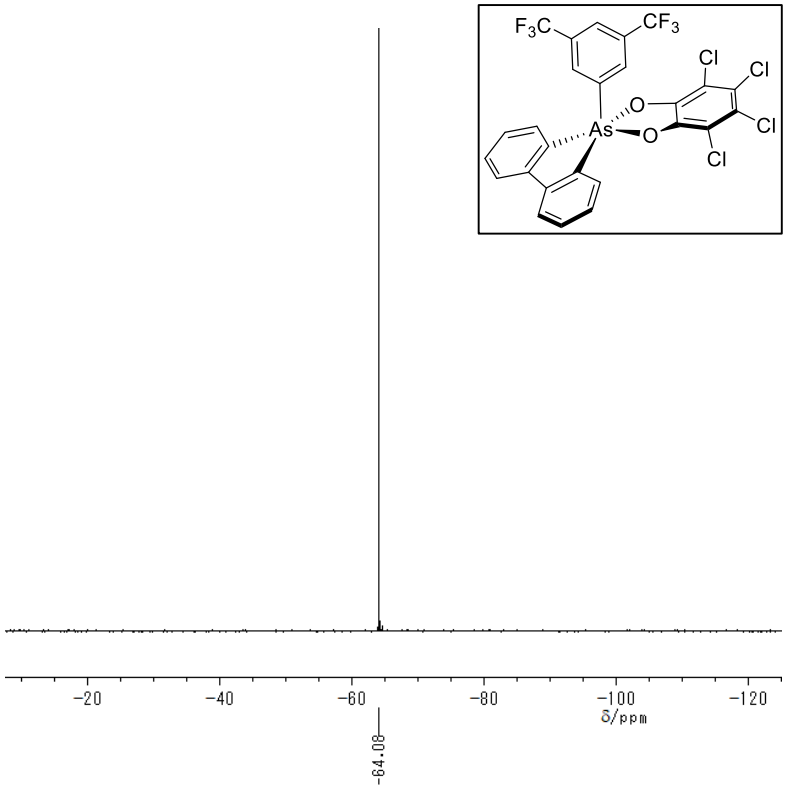


Figure S11. ^{19}F-NMR (376 MHz) spectrum for **5** in $CDCl_3$.

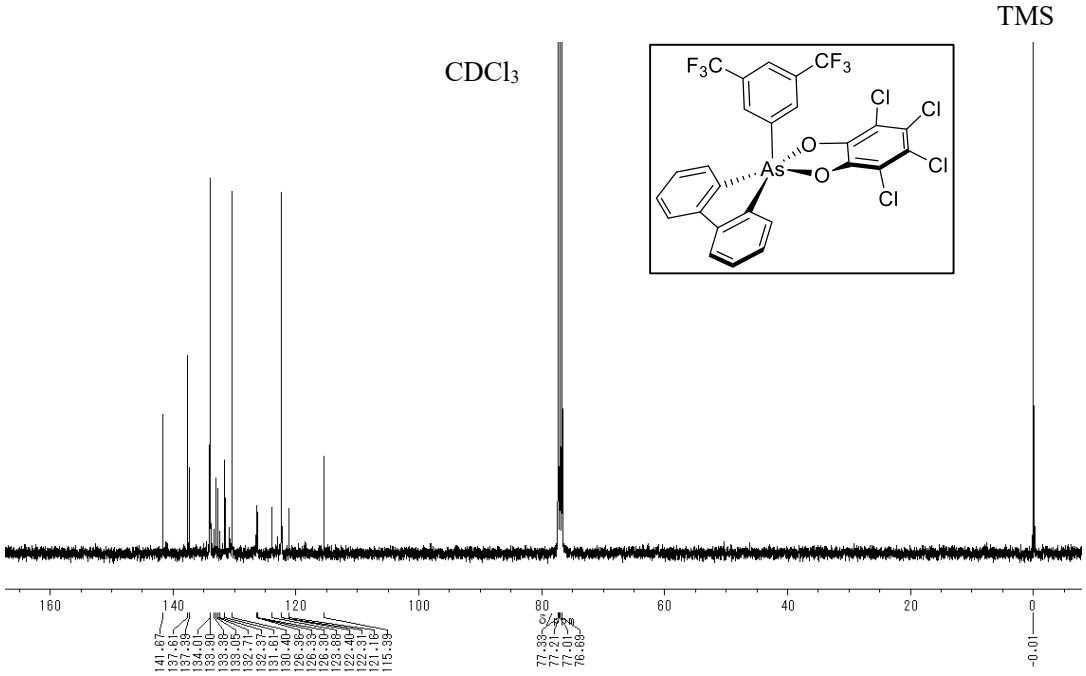


Figure S12. ^{13}C-NMR (100 MHz) spectrum for **5** in $CDCl_3$.

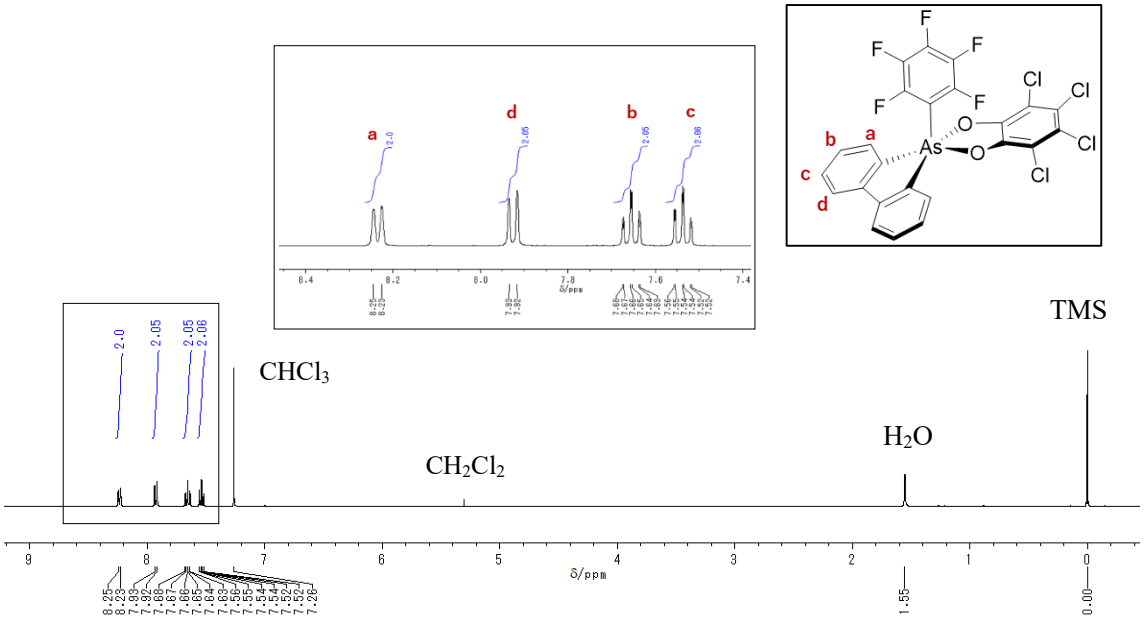


Figure S13. ^{1}H-NMR (400 MHz) spectrum for **6** in $CDCl_3$.

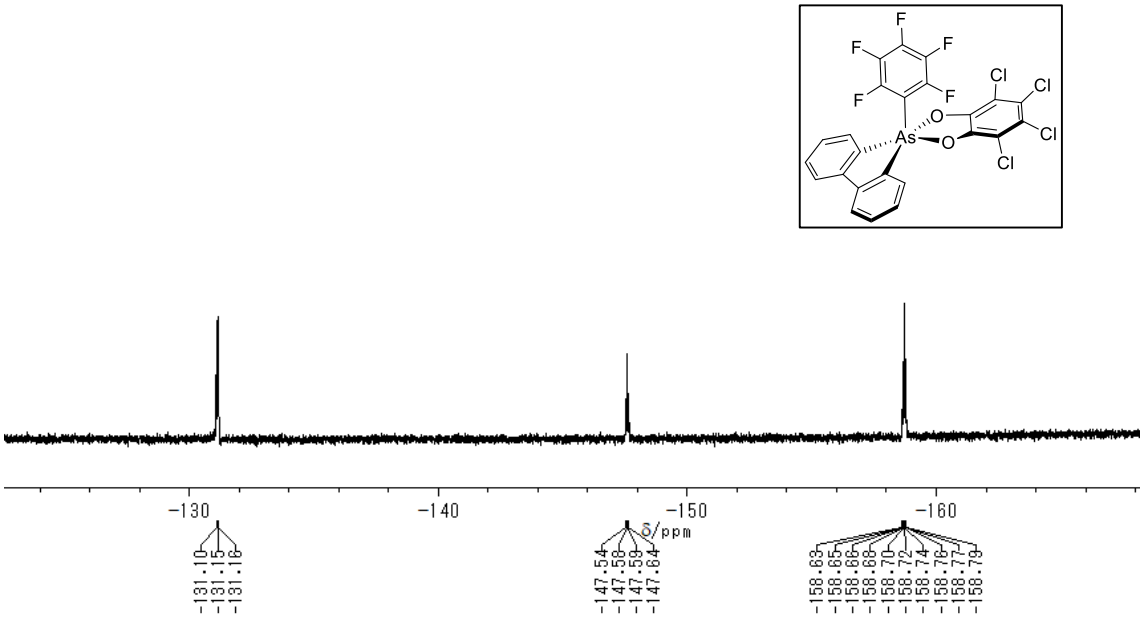


Figure S14. ^{19}F-NMR (376 MHz) spectrum for **6** in $CDCl_3$.

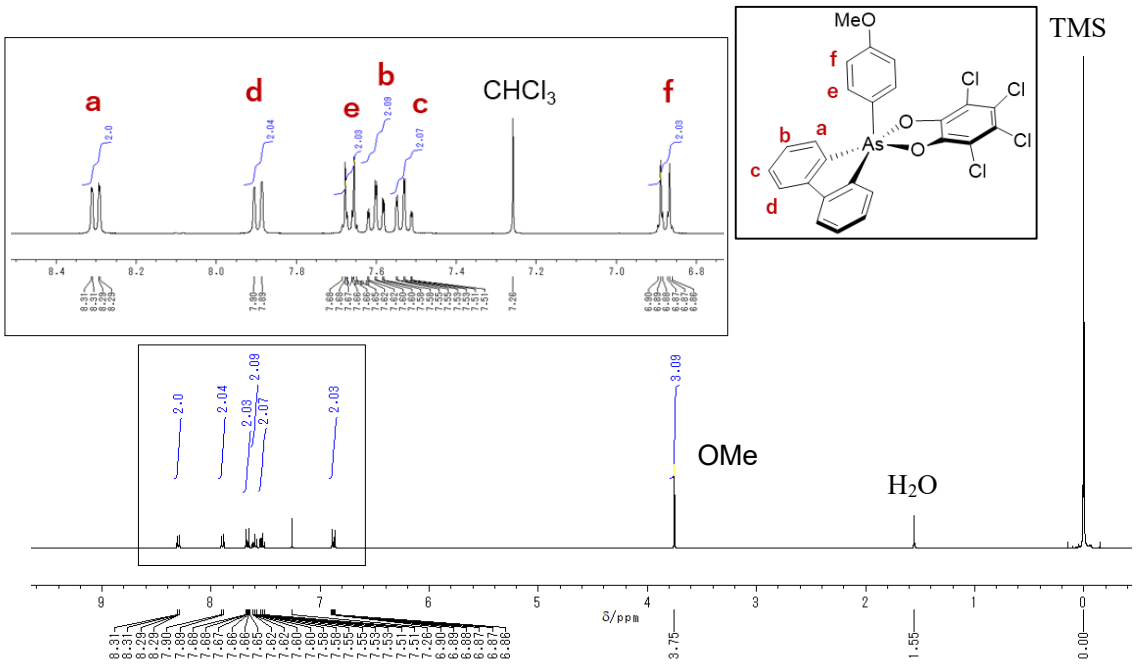


Figure S15. ^{1}H-NMR (400 MHz) spectrum for **7** in $CDCl_3$.

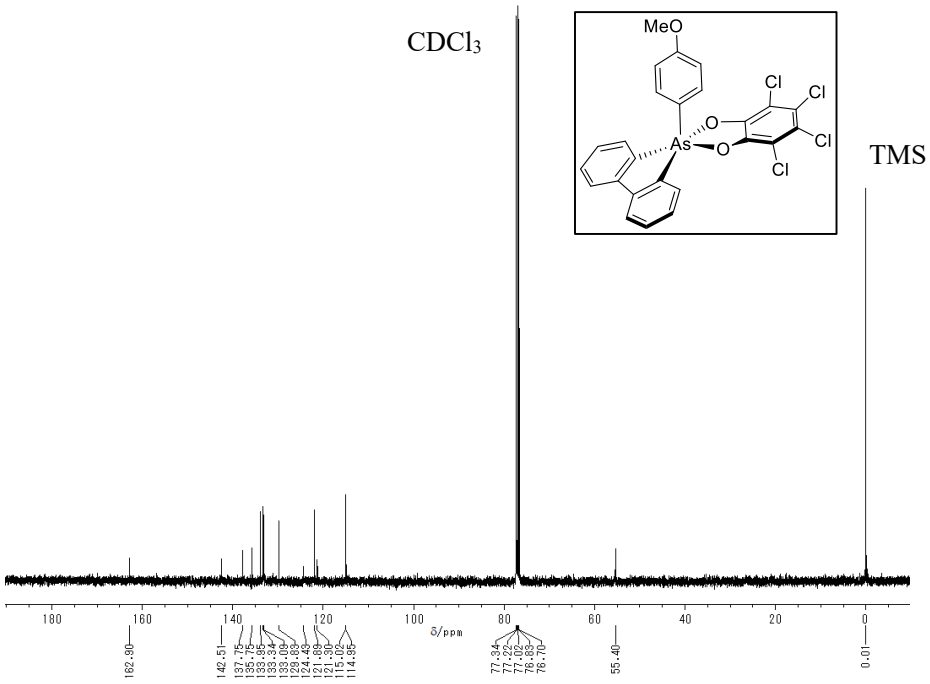


Figure S16. ^{13}C-NMR (100 MHz) spectrum for **7** in $CDCl_3$.

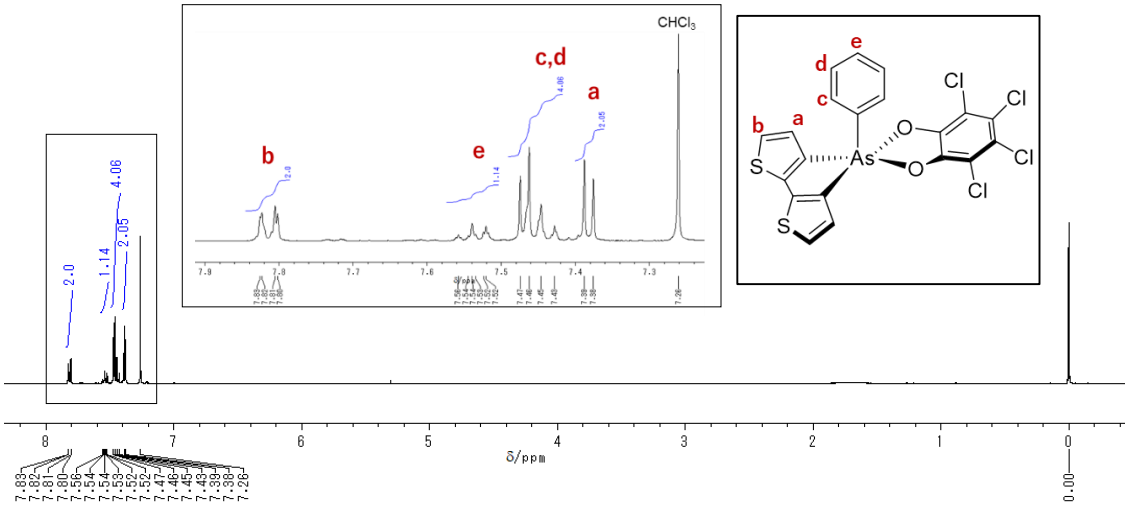


Figure S17. ^{1}H-NMR (400 MHz) spectrum for **8** in $CDCl_3$.

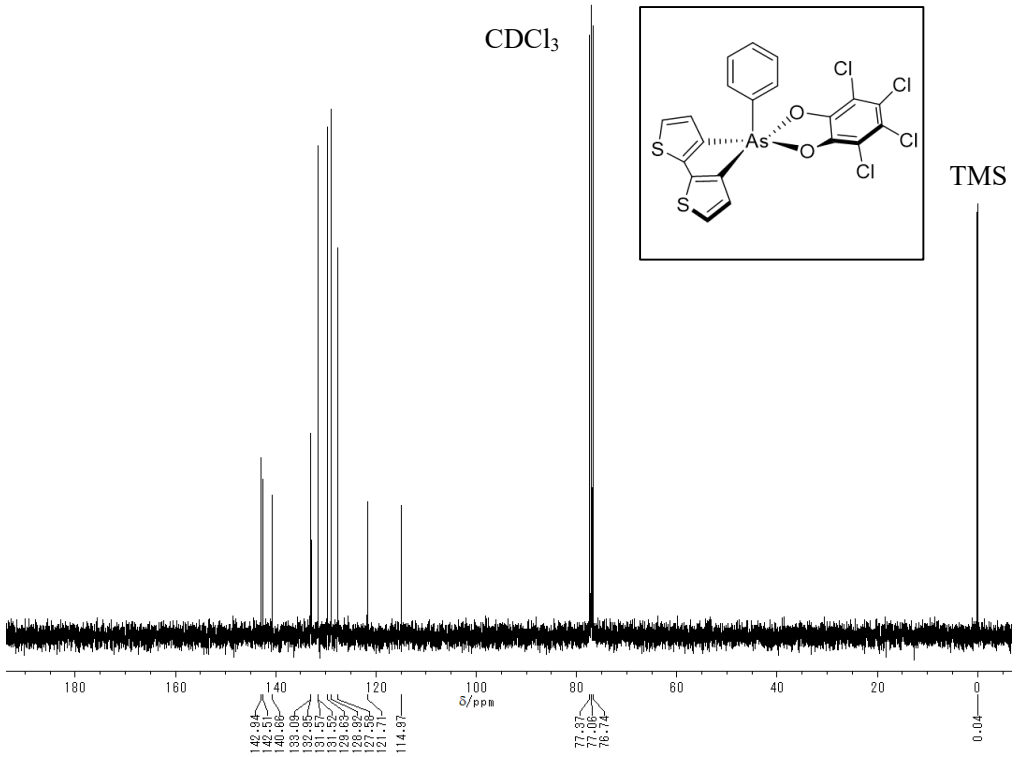


Figure S18. ^{13}C-NMR (100 MHz) spectrum for **8** in $CDCl_3$.

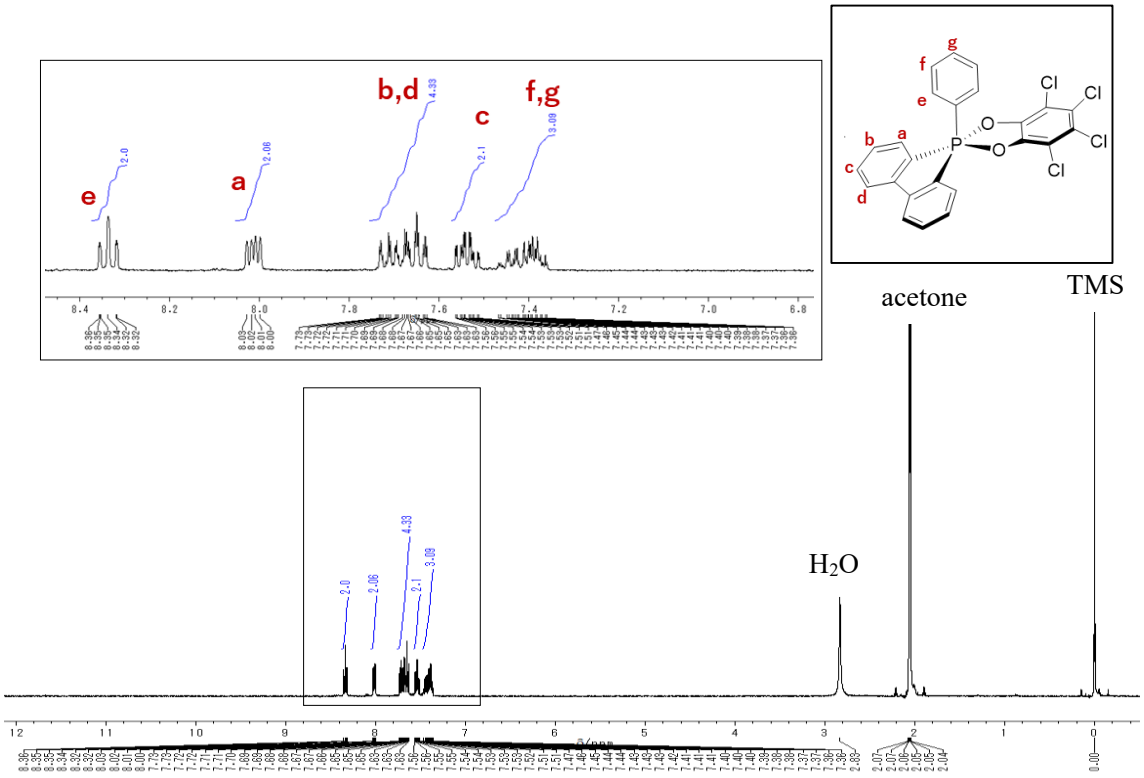


Figure S19. ^{1}H-NMR (400 MHz) spectrum for **11** in acetone-d_6.

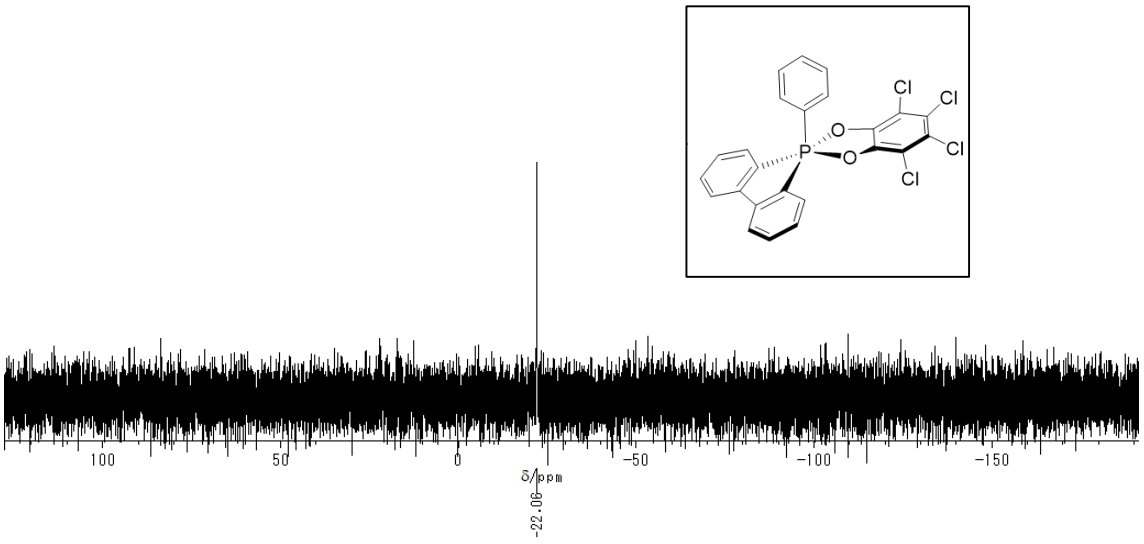


Figure S20. ^{31}P-NMR (162 MHz) spectrum for **11** in acetone-d_6.

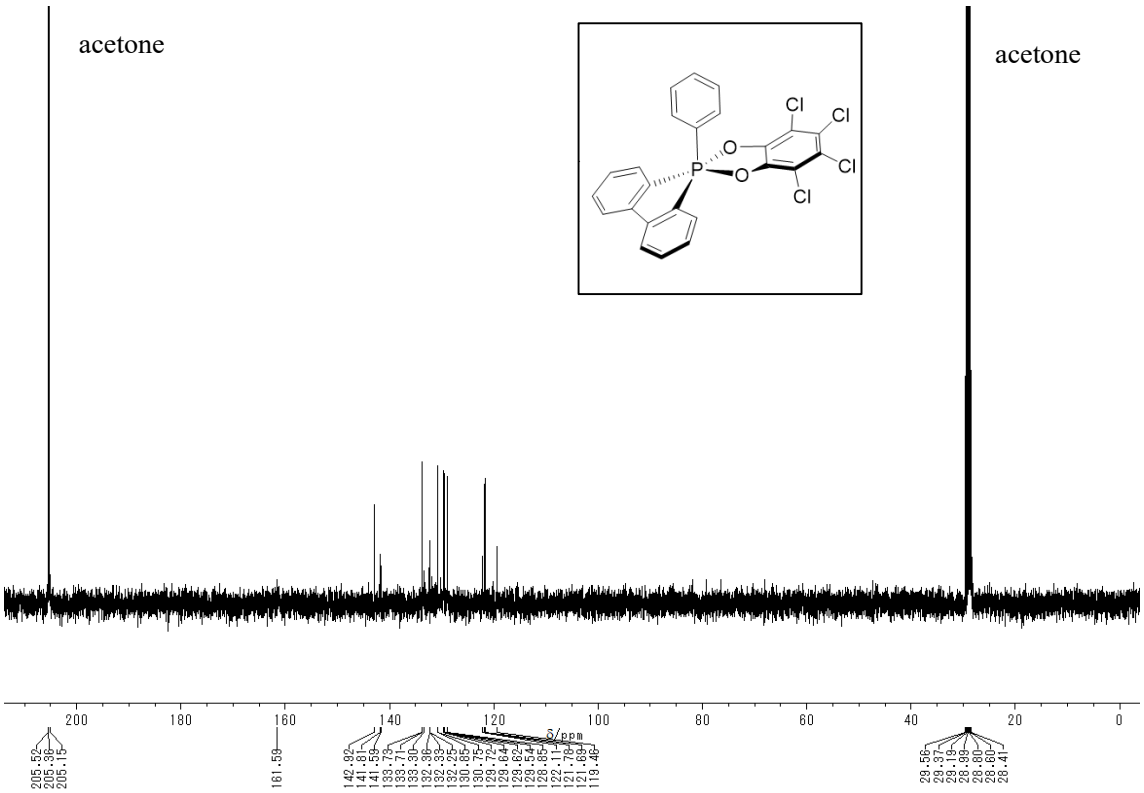


Figure S21. ^{13}C-NMR (100 MHz) spectrum for **11** in acetone-d_6.

2. Crystallographic data

Table S1. Crystallographic data of **1**, **2**, and **3**.

	1	**2**	**3**
Crystal data			
Empirical Formula	$C_{24}H_{15}AsCl_4O_2$	$C_{30}H_9AsCl_4F_{18}O_2$	$C_{54}H_{42}As_2Cl_8O_{10}$
Formula Weight	552.08	960.09	1284.31
Crystal Dimension, mm^3	0.91 × 0.53 × 0.25	0.45× 0.35 × 0.31	0.687 × 0.393 × 0.27
Crystal System	triclinic	monoclinic	triclinic
Space Group	*P*-1	$P2_1/n$	*P*-1
a, Å	9.4381(7)	10.6976(4)	10.0471(3)
b, Å	10.9659(8)	23.821(1)	12.8490(5)
c, Å	11.5914(6)	13.1719(6)	21.2792(7)
α, deg.	79.380(5)	-	92.495(3)
β, deg.	83.286(5)	92.048(4)	97.124(3)
γ, deg.	70.007(6)	-	99.593(3)
Volume, $Å^3$	1106.2(1)	3354.5(3)	2681.9(2)
D_{calcd}, g cm^{-3}	1.658	1.901	1.590
Z	2	4	2
F(000)	552.0	1872.0	1296.0
Data Collection			
Temperature, deg.	-180.0	-180.0	-180.0
2θmax, deg.	52.744	52.746	52.744
Tmin/Tmax	0.583 / 0.836	0.470 / 0.522	0.020 / 0.100
Refinement			
No. of Observed Data	4522	6856	10965
No. of Parameters	280	496	673
R1[a], wR2[b]	0.0349, 0.0889	0.0533, 0.1442	0.0568, 0.1599
Goodness of Fit Indictor	1.031	1.035	1.056

[a]$R1 = \Sigma \mid |Fo| - |Fc| \mid / \Sigma |Fo|$ [b]$wR2 = [\ \Sigma w ((Fo^2-Fc^2)^2 / \Sigma w (Fo^2)^2\ ]^{1/2}$ $w = [\ \sigma^2(Fo^2)\ ]^{-1}$

CCDC #2156251 (**1**), 2156252 (**2**), 2156253 (**3**)

Table S2. Crystallographic data of **4**, **5**, and **6**.

	4	**5**	**6**
Crystal data			
Empirical Formula	$C_{24}H_{13}AsCl_4O_2$	$C_{24}H_{11}AsCl_4F_6O_2$	$C_{24}H_8AsCl_4F_5O_2$
Formula Weight	550.10	686.07	640.02
Crystal Dimension, mm^3	0.17 × 0.10 × 0.05	0.69 × 0.37 × 0.15	0.21 × 0.16 × 0.13
Crystal System	triclinic	triclinic	monoclinic
Space Group	*P*-1	*P*-1	$P2_1/c$
a, Å	9.2905(5)	8.7605(2)	18.5696(11)
b, Å	14.1453(18)	9.4518(2)	16.0085(5)
c, Å	17.0807(10)	16.2259(3)	17.3520(11)
α, deg.	86.897(19)	105.744(2)	-
β, deg.	77.83(2)	99.000(2)	117.110(8)
γ, deg.	79.292(15)	99.061(2)	-
Volume, $Å^3$	2155.8(4)	1248.65(5)	4591.5(5)
D_{calcd}, g cm^{-3}	1.695	1.825	1.852
Z	4	2	8
F(000)	1096.0	676.0	2512.0
Data Collection			
Temperature, deg.	-180.0	-180.0	-180.0
2θmax, deg.	55.0	52.7	53.5
Tmin/Tmax	0.750 / 0.901	0.226 / 0.638	0.407 / 1.000
Refinement			
No. of Observed Data	9549	5106	9396
No. of Parameters	559	352	650
R1[a], wR2[b]	0.0479, 0.0971	0.0258, 0.0670	0.0544, 0.1443
Goodness of Fit Indictor	1.081	1.047	0.931

[a]$R1 = \Sigma \mid |Fo| - |Fc| \mid / \Sigma |Fo|$ [b]$wR2 = [\ \Sigma\ w\ ((Fo^2-Fc^2)^2 / \Sigma\ w\ (Fo^2)^2\ ]^{1/2}$ $w = [\ \sigma^2(Fo^2)\ ]^{-1}$

CCDC #2156254 (**4**), 2156258 (**5**), 2156257 (**6**)

Table S3. Crystallographic data of **7**, **8**, and **9**.

	7	**8**	**9**
Crystal data			
Empirical Formula	$C_{25}H_{15}AsCl_4O_3$	$C_{20}H_9AsCl_4O_2S_2$	$C_{24}H_{15}Cl_4O_2P$
Formula Weight	580.09	562.11	508.13
Crystal Dimension, mm^3	0.43× 0.4 × 0.37	0.63 × 0.51 × 0.24	1× 0.8 × 0.6
Crystal System	monoclinic	triclinic	triclinic
Space Group	$P2_1/n$	P-1	P-1
a, Å	8.7641(3)	8.8878(5)	8.797(1)
b, Å	16.2724(6)	10.6388(4)	9.0423(9)
c, Å	15.7928(5)	12.0109(5)	16.302(2)
α, deg.	-	106.101(3)	74.533(9)
β, deg.	94.801(3)	103.786(4)	86.78(1)
γ, deg.	-	98.692(4)	62.57(1)
Volume, $Å^3$	2244.4(1)	1030.60(9)	1106.0(2)
D_{calcd}, g cm^{-3}	1.717	1.811	1.526
Z	4	2	2
F(000)	1160.0	556.0	516.0
Data Collection			
Temperature, deg.	-180.0	-180.0	20.0
2θmax, deg.	52.738	52.744	52.744
Tmin/Tmax	0.854 / 0.884	0.569 / 0.783	0.261 / 0.504
Refinement			
No. of Observed Data	4569	4195	4521
No. of Parameters	300	262	280
R1[a], wR2[b]	0.0241, 0.0592	0.0256, 0.0624	0.0483, 0.1346
Goodness of Fit Indictor	1.046	1.039	1.066

[a]$R1 = \Sigma \mid |Fo| - |Fc| \mid / \Sigma |Fo|$ [b]$wR2 = [\ \Sigma\ w\ ((Fo^2-Fc^2)^2 / \Sigma\ w\ (Fo^2)^2\ ]^{1/2}$ $w = [\ \sigma^2(Fo^2)\ ]^{-1}$

CCDC #2156255 (**7**), 2156262 (**8**), 2156256 (**9**)

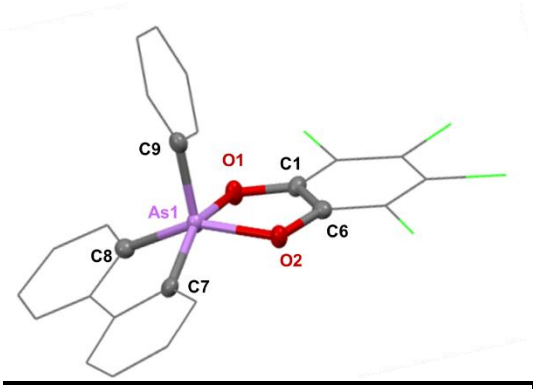
Table S4. Crystallographic data of **10**, **11**, and **12**.

	10	**11**	**12**
Crystal data			
Empirical Formula	$C_{24}H_{15}Cl_4O_2Sb$	$C_{24}H_{13}Cl_4O_2P$	$C_{24}H_{13}Cl_4O_2Sb$
Formula Weight	598.91	506.11	596.89
Crystal Dimension, mm^3	1 × 0.8× 0.38	0.479 × 0.457 × 0.236	0.22 × 0.22 × 0.09
Crystal System	monoclinic	triclinic	monoclinic
Space Group	$P2_1/n$	P-1	$C2/c$
a, Å	10.3586(7)	9.3999(8)	21.6414(7)
b, Å	10.8901(9)	13.508(1)	16.1963(6)
c, Å	21.116(1)	17.344(2)	25.843(1)
α, deg.	-	89.651(7)	-
β, deg.	102.404(6)	85.511(7)	96.869(3)
γ, deg.	-	84.269(7)	-
Volume, $Å^3$	2326.4(3)	2184.5(3)	8993.2(6)
D_{calcd}, g cm^{-3}	1.710	1.658	1.763
Z	4	4	16
F(000)	1176.0	1024.0	4672.0
Data Collection			
Temperature, deg.	20.0	20.0	20.0
2θmax, deg.	52.742	52.744	52.742
Tmin/Tmax	0.993 / 0.997	0.838 / 0.918	0.999 / 0.999
Refinement			
No. of Observed Data	4733	8934	9183
No. of Parameters	280	559	559
R1[a], wR2[b]	0.0328, 0.0860	0.0620, 0.2090	0.0302, 0.0740
Goodness of Fit Indictor	1.119	0.995	1.002

[a] $R1 = \Sigma \mid |Fo| - |Fc| \mid / \Sigma |Fo|$ [b] $wR2 = [\ \Sigma\ w\ ((Fo^2-Fc^2)^2 / \Sigma\ w\ (Fo^2)^2\ ]^{1/2}$ $w = [\ \sigma^2(Fo^2)\ ]^{-1}$

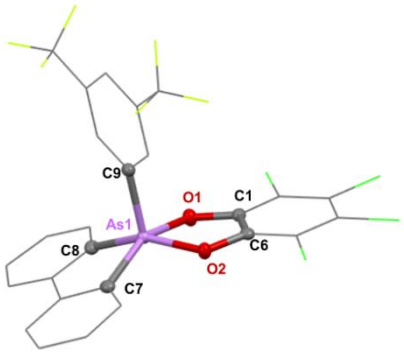
CCDC #2156260 (**10**), 2156259 (**11**), 2156261 (**12**)

Table S5. ORTEP drawing (ellipsoids at 50% probability), selected distances, and angles of **4**. Hydrogen atoms were omitted for clarity.



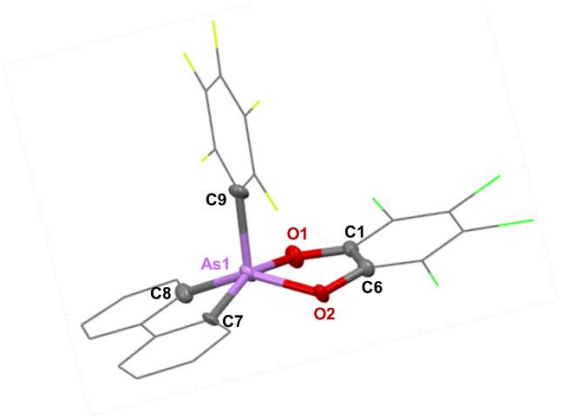
distances (Å)				angles (°)			
As1-C7	1.937(4)	As1-O2	1.877(3)	C8-As1-C7	88.0(2)	C8-As1-C9	110.7(2)
As1-C8	1.942(4)	C6-C1	1.400(6)	C7-As1-O2	87.9(1)	C8-As1-O2	148.3(1)
As1-C9	1.930(3)	O1-C1	1.344(4)	O2-As1-O1	83.6(1)	C7-As1-O1	154.5(1)
As1-O1	1.917(3)	O2-C6	1.357(5)	O1-As1-C8	86.7(1)		

Table S6. ORTEP drawing (ellipsoids at 50% probability), selected distances, and angles of **5**. Hydrogen atoms were omitted for clarity.



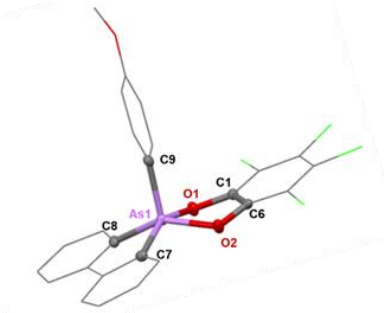
distances (Å)				angles (°)			
As1-C7	1.943(2)	As1-O2	1.902(1)	C8-As1-C7	88.23(8)	C8-As1-C9	104.86(8)
As1-C8	1.941(2)	C6-C1	1.397(2)	C7-As1-O2	88.88(7)	C8-As1-O2	156.60(7)
As1-C9	1.938(2)	O1-C1	1.346(2)	O2-As1-O1	83.96(6)	C7-As1-O1	153.78(7)
As1-O1	1.881(1)	O2-C6	1.351(2)	O1-As1-C8	88.46(7)		

Table S7. ORTEP drawing (ellipsoids at 50% probability), selected distances, and angles of **6**. Hydrogen atoms were omitted for clarity.



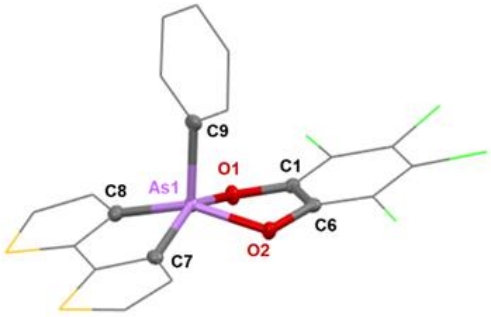
distances (Å)				angles (°)			
As1-C7	1.940(6)	As1-O2	1.881(6)	C8-As1-C7	89.1(3)	C8-As1-C9	108.5(3)
As1-C8	1.935(7)	C6-C1	1.369(9)	C7-As1-O2	88.3(3)	C8-As1-O2	148.3(3)
As1-C9	1.944(8)	O1-C1	1.33(1)	O2-As1-O1	83.2(2)	C7-As1-O1	158.6(3)
As1-O1	1.905(4)	O2-C6	1.360(8)	O1-As1-C8	88.0(3)		

Table S8. ORTEP drawing (ellipsoids at 50% probability), selected distances, and angles of **7**. Hydrogen atoms were omitted for clarity.



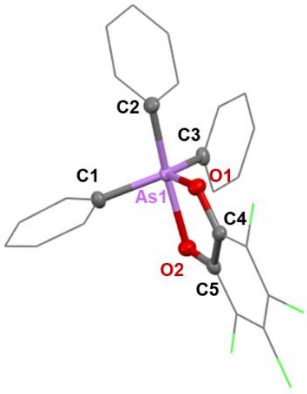
distances (Å)				angles (°)			
As1-C7	1.941(2)	As1-O2	1.897(1)	C8-As1-C7	88.16(8)	C8-As1-C9	108.16(8)
As1-C8	1.935(2)	C6-C1	1.399(3)	C7-As1-O2	87.38(7)	C8-As1-O2	149.50(7)
As1-C9	1.908(2)	O1-C1	1.342(2)	O2-As1-O1	82.36(6)	C7-As1-O1	153.45(7)
As1-O1	1.923(1)	O2-C6	1.345(2)	O1-As1-C8	88.41(7)		

Table S9. ORTEP drawing (ellipsoids at 50% probability), selected distances, and angles of **8**. Hydrogen atoms were omitted for clarity.



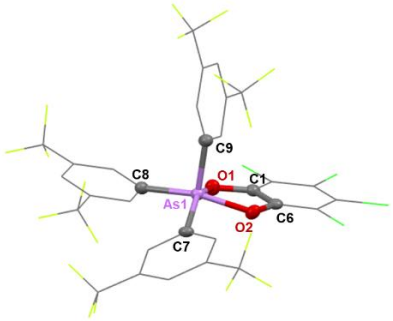
distances (Å)				angles (°)			
As1-C7	1.944(2)	As1-O2	1.909(2)	C8-As1-C7	87.56(8)	C8-As1-C9	107.82(9)
As1-C8	1.942(2)	C6-C1	1.403(3)	C7-As1-O2	88.06(7)	C8-As1-O2	154.07(8)
As1-C9	1.925(2)	O1-C1	1.350(2)	O2-As1-O1	83.04(6)	C7-As1-O1	149.99(8)
As1-O1	1.897(2)	O2-C6	1.347(2)	O1-As1-C8	88.10(8)		

Table S10. ORTEP drawing (ellipsoids at 50% probability), selected distances, and angles of **1**. Hydrogen atoms were omitted for clarity.



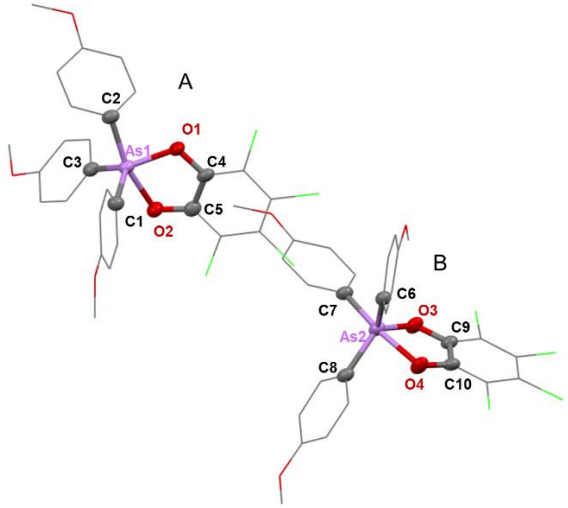
distances (Å)				angles (°)			
As1-C1	1.926(3)	As1-O2	2.068(2)	C1-As1-O1	116.2(1)	C2-As1-O1	87.7(1)
As1-C2	1.969(3)	C5-C4	1.403(3)	O1-As1-C3	123.8(1)	C2-As1-C3	99.9(1)
As1-C3	1.945(3)	O1-C4	1.367(3)	C3-As1-C1	116.8(1)	C2-As1-O2	169.4(1)
As1-O1	1.824(2)	O2-C5	1.322(3)	C1-As1-C2	100.6(1)	O1-As1-O2	81.67(8)

Table S11. ORTEP drawing (ellipsoids at 50% probability), selected distances, and angles of **2**. Hydrogen atoms were omitted for clarity.



distances (Å)				angles (°)			
As1-C7	1.966(4)	As1-O2	1.920(3)	C8-As1-C7	98.7(2)	C8-As1-C9	100.1(2)
As1-C8	1.975(4)	C6-C1	1.386(6)	C7-As1-O2	84.9(1)	C8-As1-O2	161.0(1)
As1-C9	1.937(4)	O1-C1	1.352(5)	O2-As1-O1	83.3(1)	C7-As1-O1	147.5(1)
As1-O1	1.862(2)	O2-C6	1.347(5)	O1-As1-C8	83.9(1)		

Table S12. ORTEP drawing (ellipsoids at 50% probability), selected distances, and angles of **3**. Hydrogen atoms were omitted for clarity.



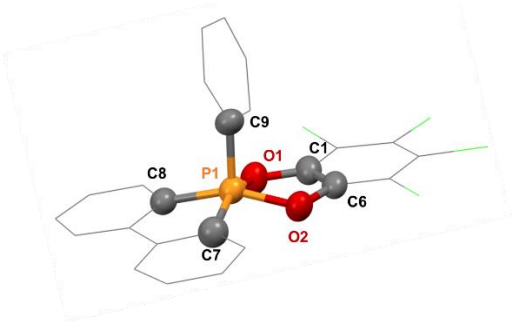
A

distances (Å)				angles (°)			
As1-C1	1.914(4)	As1-O2	2.083(3)	C1-As1-O1	110.8(1)	C2-As1-O1	86.6(1)
As1-C2	1.948(4)	C5-C4	1.411(6)	O1-As1-C3	130.9(1)	C2-As1-C3	99.2(2)
As1-C3	1.922(4)	O1-C4	1.372(4)	C3-As1-C1	114.8(2)	C2-As1-O2	162.7(1)
As1-O1	1.838(3)	O2-C5	1.308(5)	C1-As1-C2	103.7(2)	O1-As1-O2	80.1(1)

B

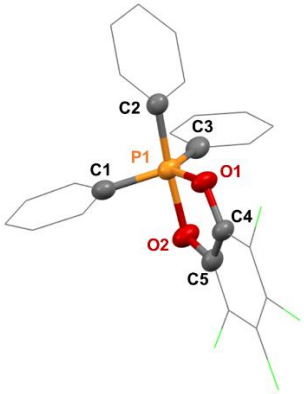
distances (Å)				angles (°)			
As2-C6	1.909(4)	As2-O4	2.107(3)	C6-As2-O3	117.8(1)	C7-As2-O3	89.4(1)
As2-C7	1.949(4)	C10-C9	1.405(6)	O3-As2-C8	116.5(1)	C7-As2-C8	100.9(2)
As2-C8	1.917(4)	O3-C9	1.356(5)	C8-As2-C6	121.9(2)	C7-As2-O4	170.6(1)
As2-O3	1.820(2)	O4-C10	1.311(4)	C6-As2-C7	98.8(2)	O3-As2-O4	81.2(1)

Table S13. ORTEP drawing (ellipsoids at 50% probability), selected distances, and angles of **11**. Hydrogen atoms were omitted for clarity.



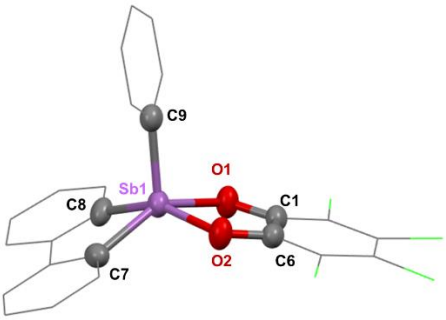
distances (Å)				angles (°)			
P1-C7	1.827(5)	P1-O2	1.739(3)	C8-P1-C7	89.5(2)	C8-P1-C9	104.3(2)
P1-C8	1.856(4)	C6-C1	1.372(6)	C7-P1-O2	86.6(2)	C8-P1-O2	155.9(2)
P1-C9	1.795(4)	O1-C1	1.358(4)	O2-P1-O1	86.9(1)	C7-P1-O1	154.9(2)
P1-O1	1.737(3)	O2-C6	1.363(5)	O1-P1-C8	86.6(2)		

Table S14. ORTEP drawing (ellipsoids at 50% probability), selected distances, and angles of **9**. Hydrogen atoms were omitted for clarity.



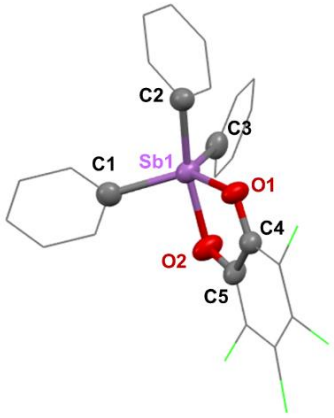
distances (Å)				angles (°)			
P1-C1	1.809(4)	P1-O2	1.916(2)	C1-P1-O1	119.8(1)	C2-P1-O1	89.6(1)
P1-C2	1.864(2)	C5-C4	1.372(4)	O1-P1-C3	120.2(1)	C2-P1-C3	95.3(1)
P1-C3	1.811(4)	O1-C4	1.375(3)	C3-P1-C1	118.4(1)	C2-P1-O2	175.0(1)
P1-O1	1.640(2)	O2-C5	1.333(3)	C1-P1-C2	97.7(1)	O1-P1-O2	85.8(1)

Table S15. ORTEP drawing (ellipsoids at 50% probability), selected distances, and angles of **12**. Hydrogen atoms were omitted for clarity.



distances (Å)				angles (°)			
Sb1-C7	2.108(3)	Sb1-O2	2.050(2)	C8- Sb1-C7	83.8(1)	C8- Sb1-C9	105.0(1)
Sb1-C8	2.117(3)	C6-C1	1.400(4)	C7- Sb1-O2	89.7(1)	C8- Sb1-O2	153.5(1)
Sb1-C9	2.093(3)	O1-C1	1.346(3)	O2- Sb1-O1	80.00(8)	C7- Sb1-O1	146.4(1)
Sb1-O1	2.028(2)	O2-C6	1.340(4)	O1- Sb1-C8	91.4(1)		

Table S16. ORTEP drawing (ellipsoids at 50% probability), selected distances, and angles of **10**. Hydrogen atoms were omitted for clarity.



distances (Å)				angles (°)			
Sb1-C1	2.122(3)	Sb1-O2	2.105(2)	C1- Sb1-O1	123.9(1)	C2- Sb1-O1	85.1(1)
Sb1-C2	2.141(4)	C5-C4	1.407(5)	O1- Sb1-C3	121.8(1)	C2- Sb1-C3	99.9(1)
Sb1-C3	2.107(4)	O1-C4	1.345(4)	C3- Sb1-C1	111.7(1)	C2- Sb1-O2	163.2(1)
Sb1-O1	2.016(2)	O2-C5	1.325(4)	C1- Sb1-C2	102.0(1)	O1- Sb1-O2	78.10(9)

3. UV-vis absorption spectra and CV data

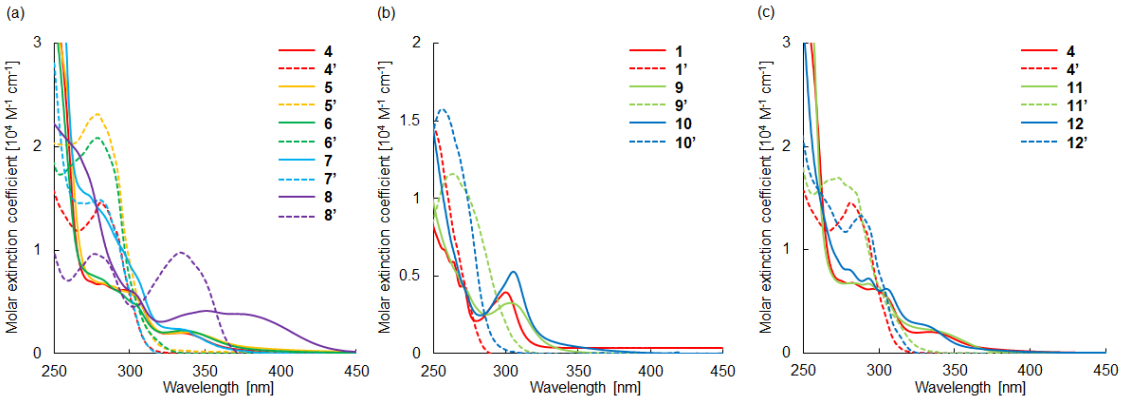


Figure S22. UV-vis absorption spectra (in CH_2Cl_2 or $CHCl_3$) of (a) **4-8** and **4'-8'**, (b) **1**, **9**, **10**, **1'**, **9'**, and **10'**, and (c) **4**, **11**, **12**, **4'**, **11'**, and **12'**

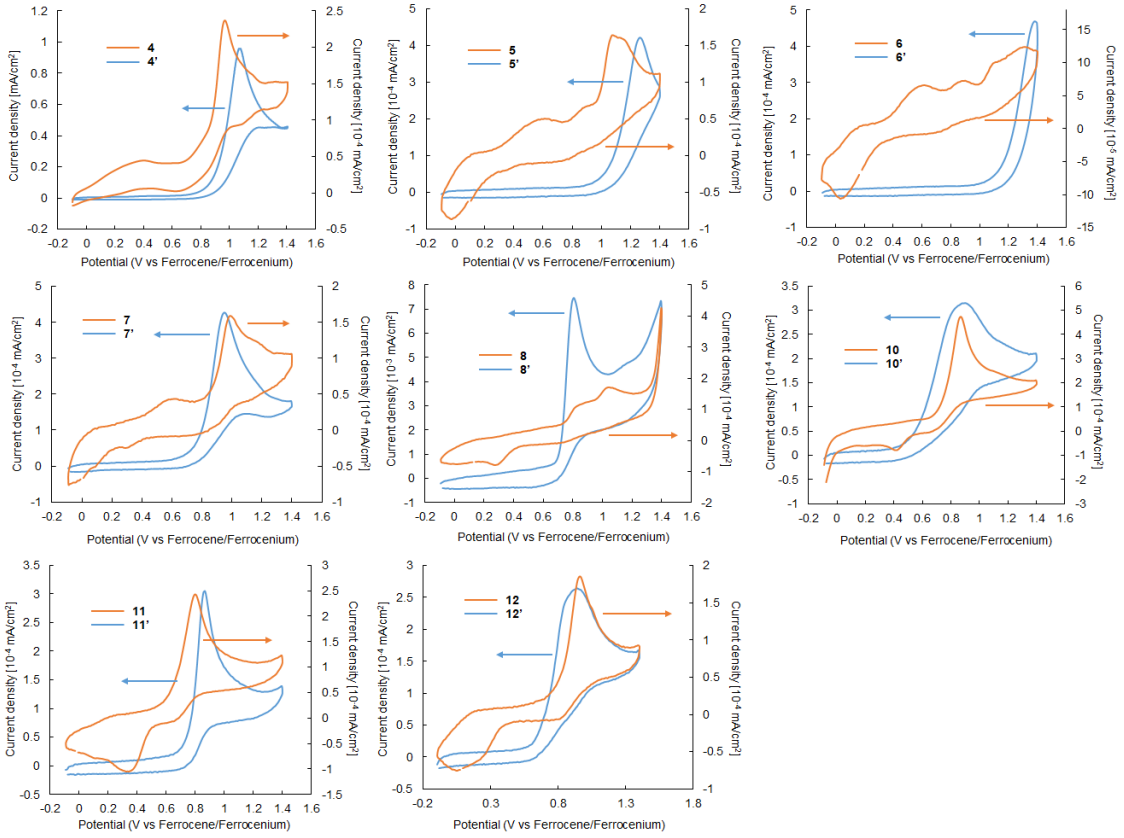


Figure S23. Cyclic voltammograms of X in 0.1 M Bu_4NPF_6/MeCN at a scan rate of 100 mV/s. X: **4** (0.5 mM), **4'** (0.5 mM), **5** (0.4 mM), **5'** (1 mM), **6** (0.4 mM), **6'** (1 mM), **7** (0.4 mM), **7'** (1 mM), **8** (0.4 mM), **8'** (1 mM), **10** (1 mM), **10'** (1 mM), **11** (0.4 mM), **11'** (1 mM), **12** (0.4 mM), and **12'** (1 mM).

Table S17. Results of UV-vis absorption measurement[a] and cyclic voltammetry[b]

	λ_{abs}[c] [nm]	E[d] [eV]	HOMO[e] [eV]	LUMO[f] [eV]		λ_{abs}[c] [nm]	E[d] [eV]	HOMO[e] [eV]	LUMO[f] [eV]
4	342	3.35	-6.20	-2.85	**4'**	281	3.99	-6.23	-2.24
5	341	3.25	-6.31	-3.06	**5'**	280	3.97	-6.44	-2.47
6	343	3.25	-6.53	-3.28	**6'**	280	3.91	-6.51	-2.60
7	337	3.32	-6.18	-2.86	**7'**	281	3.98	-6.10	-2.11
8	384	2.87	-6.02	-3.15	**8'**	335	3.38	-6.05	-2.67
10	307	3.74	-6.07	-2.33	**10'**	257	4.29	-5.84	-1.55
11	343	3.33	-5.99	-2.67	**11'**	275	3.79	-6.09	-2.30
12	340	3.42	-6.10	-2.69	**12'**	290	3.86	-6.06	-2.20

[a] Measured in CH_2Cl_2 or $CHCl_3$. [b] Measured in 0.1 M Bu_4NPF_6/MeCN (Figure S23). [c] Absorption maxima. [d] HOMO-LUMO gaps estimated by the offsets of the absorption spectra. [e] Estimated by CV (E(HOMO) = −(E_{ox} + 4.71) [eV], where E_{ox} is the onset potential of oxidation (V vs. SHE)). [f] Calculated by the HOMO-LUMO gaps (estimated by UV-vis absorption spectra) and HOMO energies (estimated by CV).

4. Determination of stoichiometry by Job plots

The total concentration of tetrachlorocatecholates and Ph_3PO were both constant and prepared in $CDCl_3$. Then various ratio of mixture solutions was added to the NMR tube. The chemical shifts due to the Ph_3PO in the ^{31}P-NMR were monitored, and the data were analyzed by using Job plots method. The association stoichiometry was obtained from the x coordinate at the maximum in the curve. The x axis is [B]/([A]+[B]) and the y axis is $|\Delta\delta|\times$[B]/([A]+[B]); $|\Delta\delta|$ means absolute value of chemical shift variation between the unassociated guest molecule and associated one, [A] and [B] means concentration of tetrachlorocatecholates and Ph_3PO.

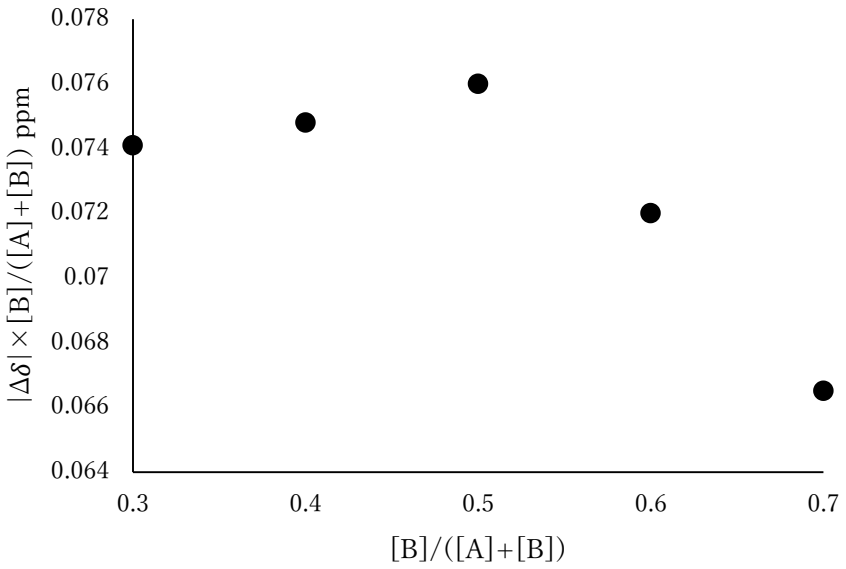


Figure S24. Job plots of **4** with PPh_3PO in $CDCl_3$, [A]+[B] = 16.0 mM.

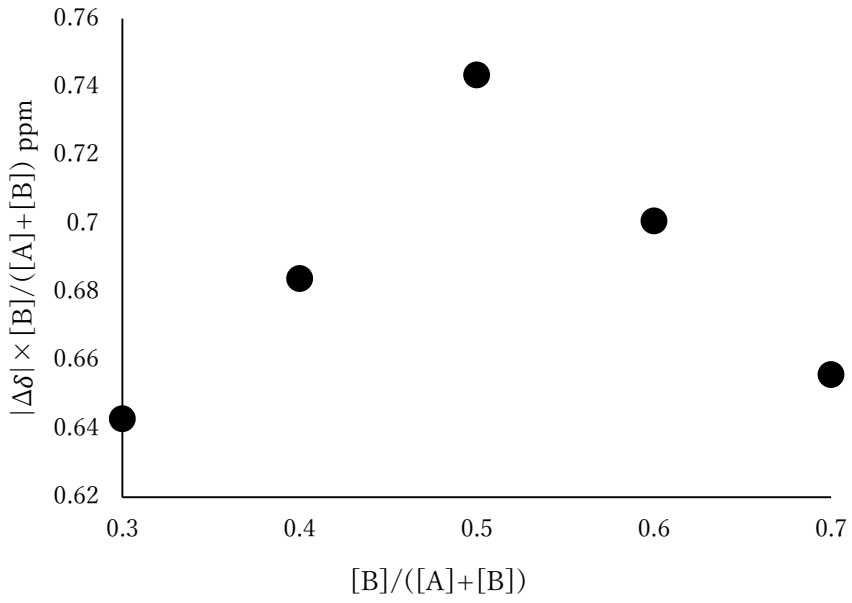


Figure S25. Job plots of **5** with PPh_3PO in $CDCl_3$, [A]+[B] = 40.0 mM.

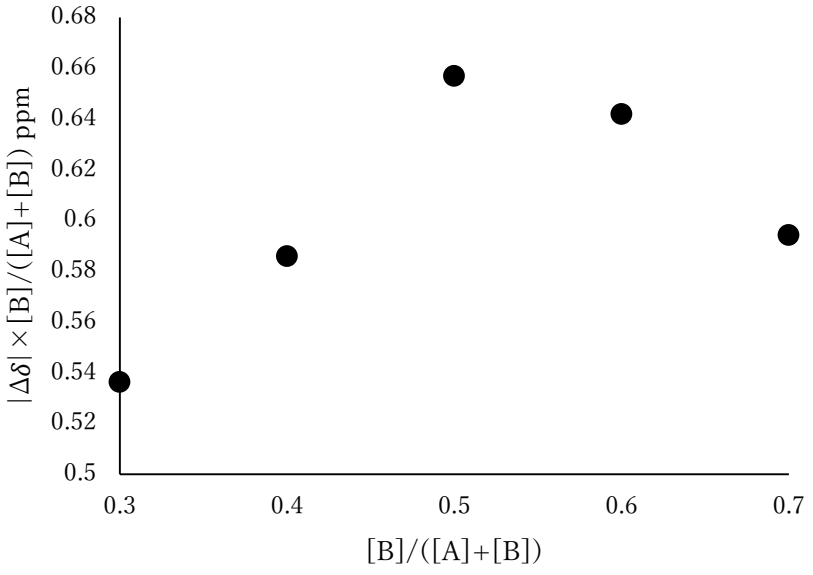


Figure S26. Job plots of **6** with PPh_3PO in $CDCl_3$, [A]+[B] = 20.0 mM.

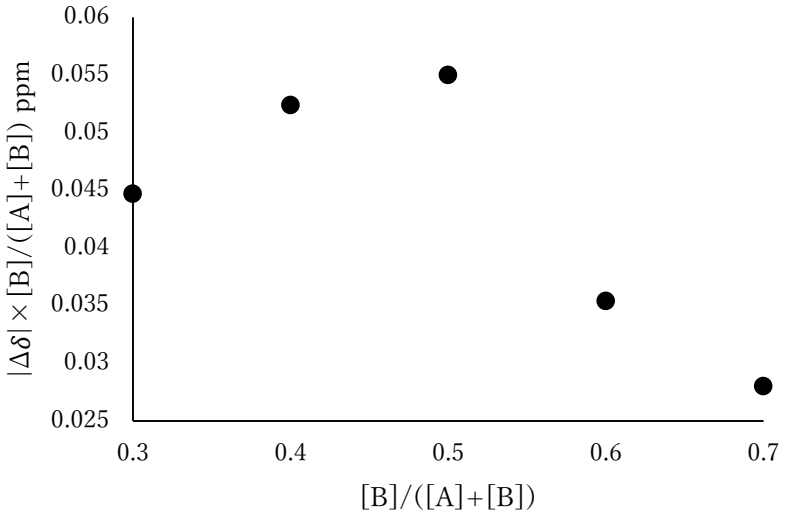


Figure S27. Job plots of **7** with PPh_3PO in $CDCl_3$, [A]+[B] = 20.0 mM.

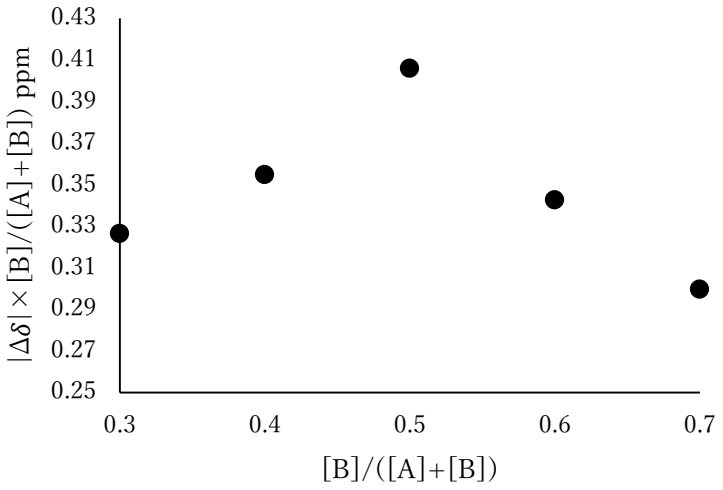


Figure S28. Job plots of **8** with PPh_3PO in $CDCl_3$, [A]+[B] = 20.0 mM.

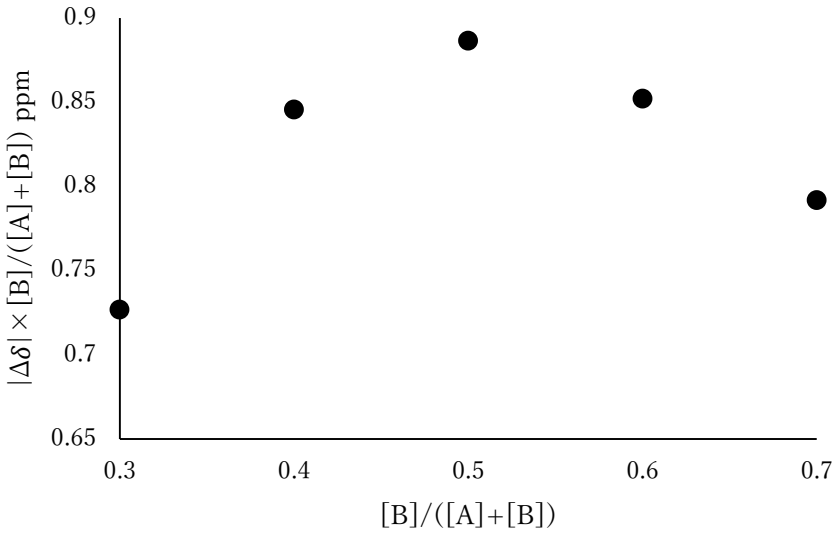


Figure S29. Job plots of **10** with PPh_3PO in $CDCl_3$, [A]+[B] = 16.0 mM.

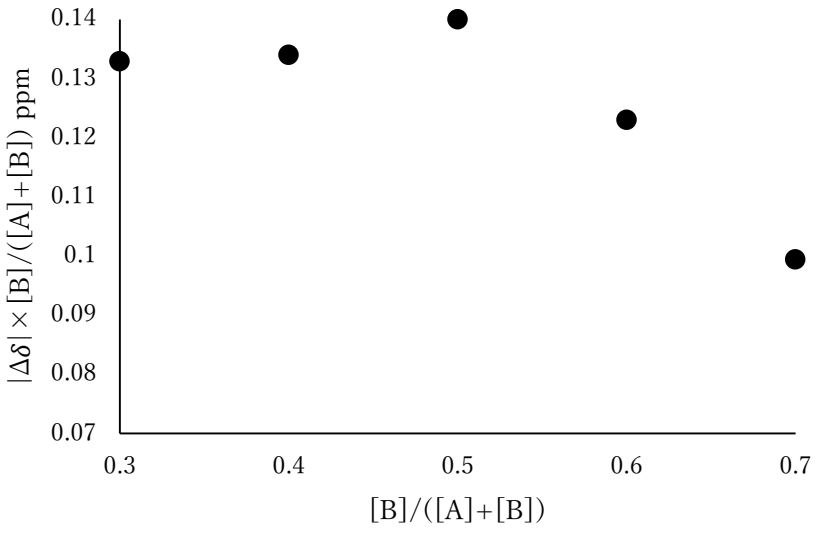


Figure S30. Job plots of **11** with PPh_3PO in $CDCl_3$, [A]+[B] = 16.0 mM.

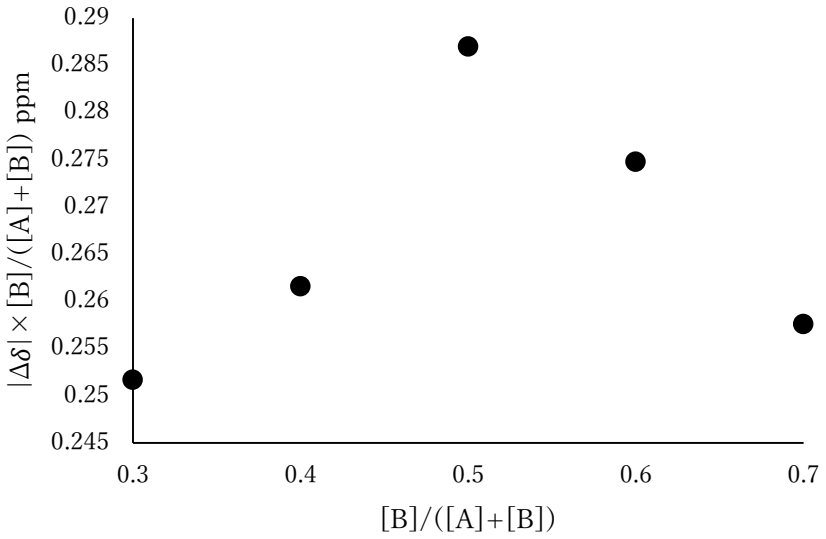


Figure S31. Job plots of **12** with PPh_3PO in $CDCl_3$, [A]+[B] = 16.0 mM.

5. Determination of association constants

Determination of the association constants for the tetrachlorocatecholates and Ph_3PO was carried out by NMR titration in $CDCl_3$. The chemical shifts due to the Ph_3PO were monitored in the ^{31}P-NMR spectra. The concentration of Ph_3PO ([B]) and solvent ratio were both constant, varied ratio of tetrachlorocatecholates ([A]). Because the host-guest complexation equilibrium has a faster exchange rate compared to the NMR time scale, association constants were determined by non- linear curve fitting analysis[1] (**1**) by down field shifting in ^{31}P-NMR.

$$|\Delta\delta| = \frac{|\Delta\delta max|}{2K[B]_0}\{1 + K[A] + K[B]_0 - [(1 + K[A] + K[B]_0)^2 - 4K^2\ [A][B]_0]^{\frac{1}{2}}\} \quad (\mathbf{1})$$

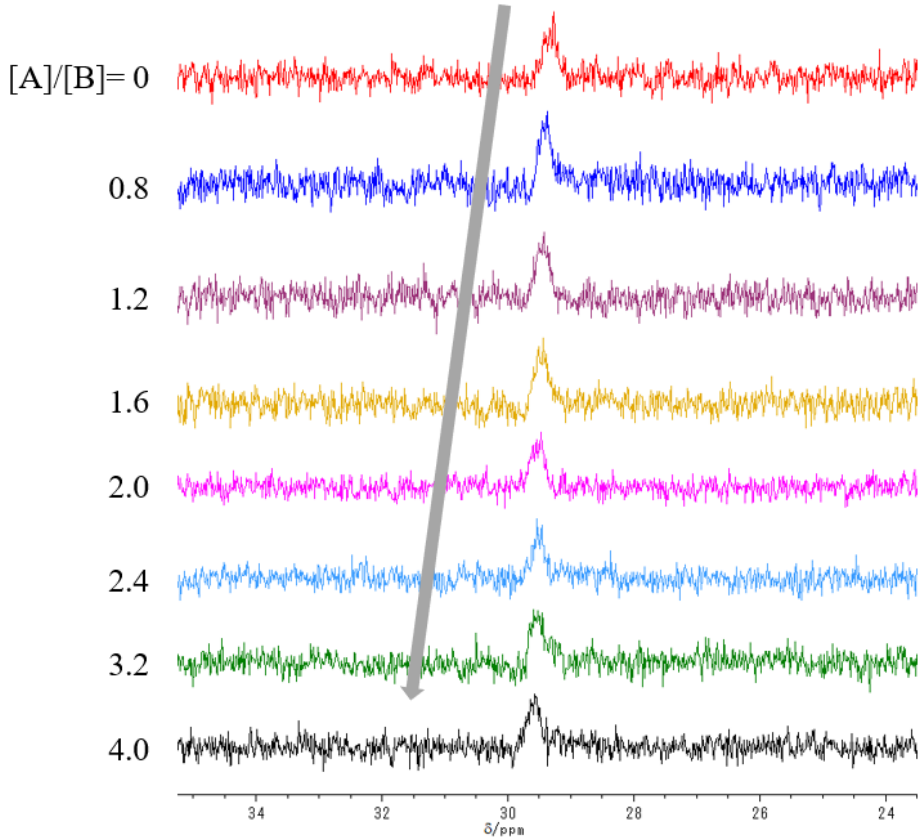


Figure S32. ^{31}P-NMR spectra of titration; PPh_3O with **4**.

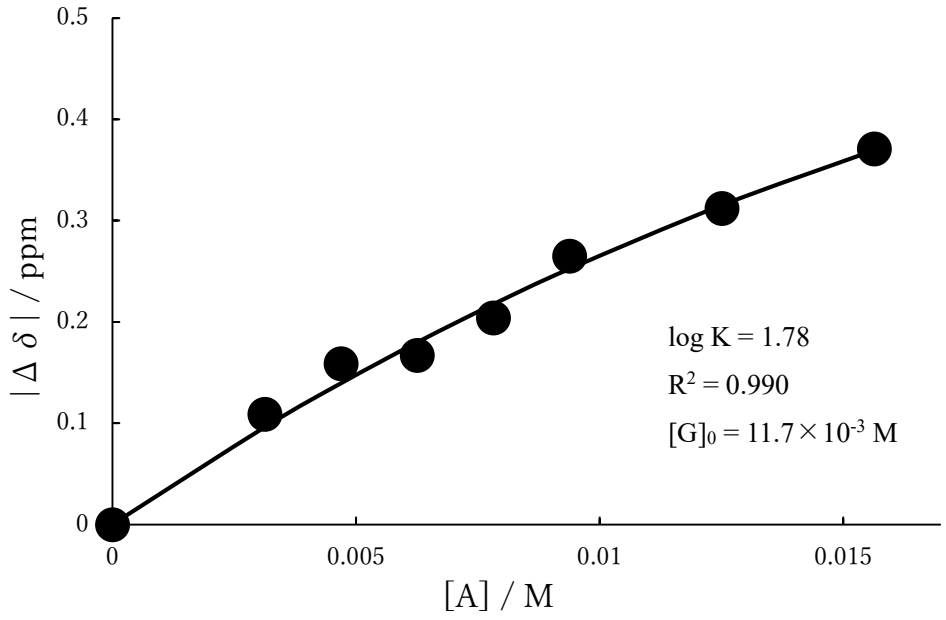


Figure S33. ^{31}P-NMR titration of PPh_3O with **4**.

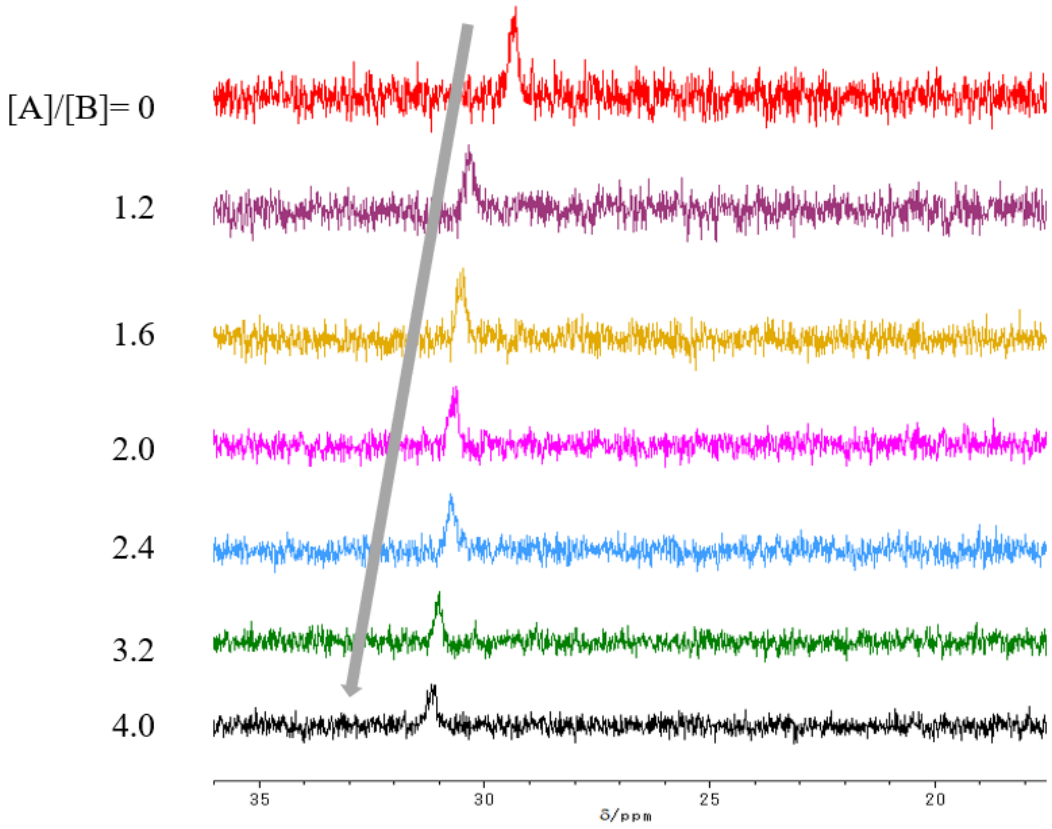


Figure S34. ^{31}P-NMR spectra of titration; PPh_3O with **5**.

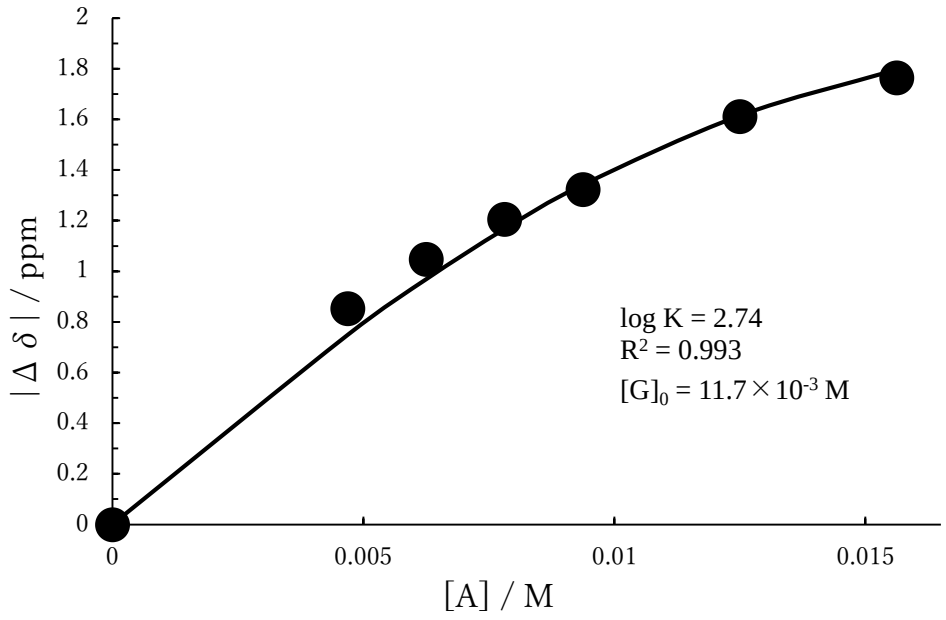


Figure S35. ^{31}P-NMR titration of PPh_3O with **5**.

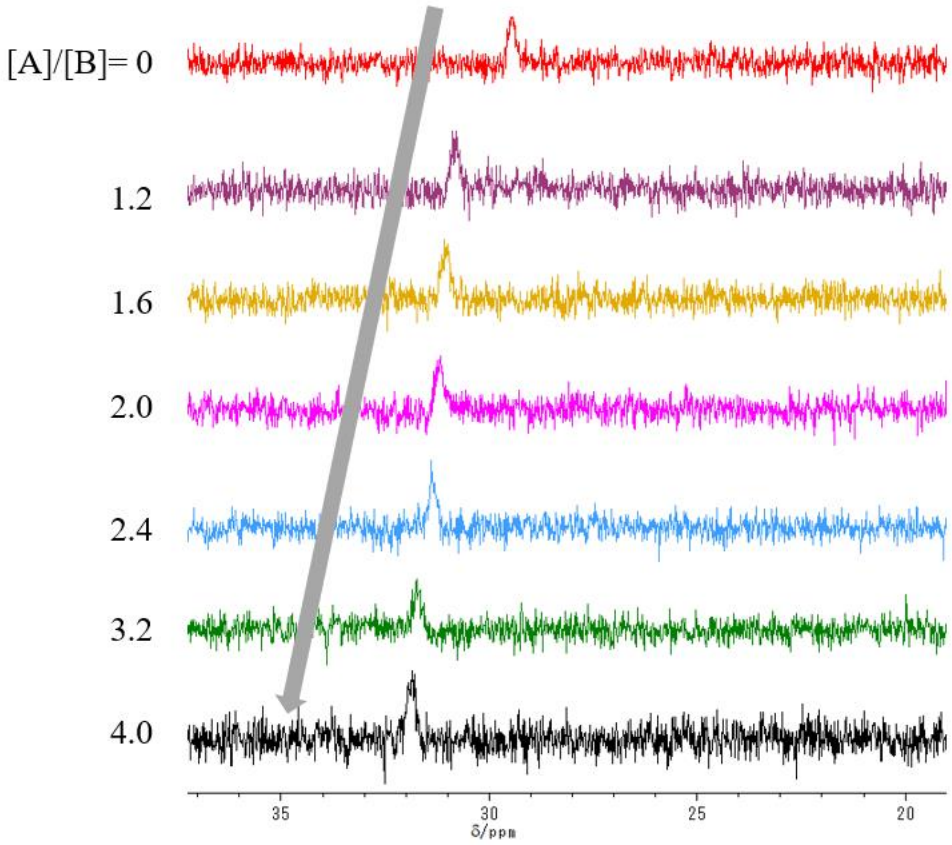


Figure S36. ^{31}P-NMR spectra of titration; PPh_3O with **6**.

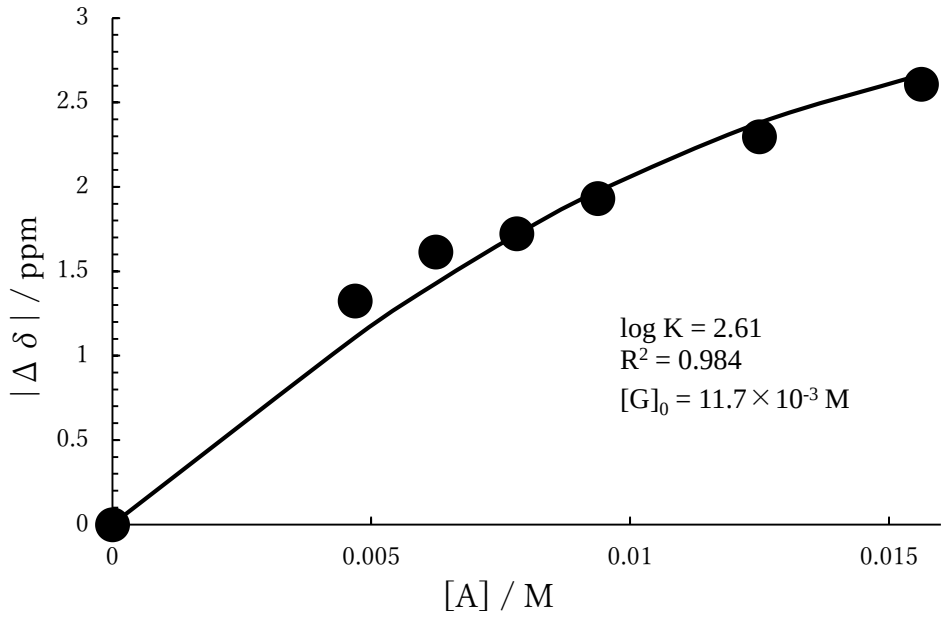


Figure S37. ^{31}P-NMR titration of PPh_3O with **6**.

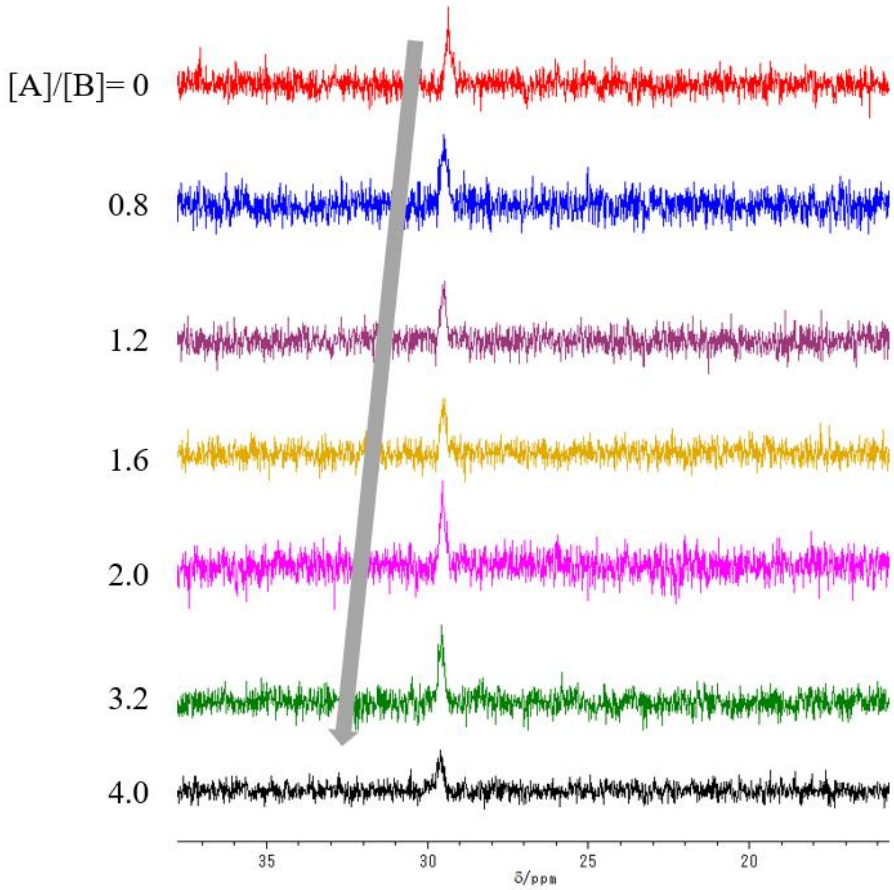


Figure S38. ^{31}P-NMR spectra of titration; PPh_3O with **7**.

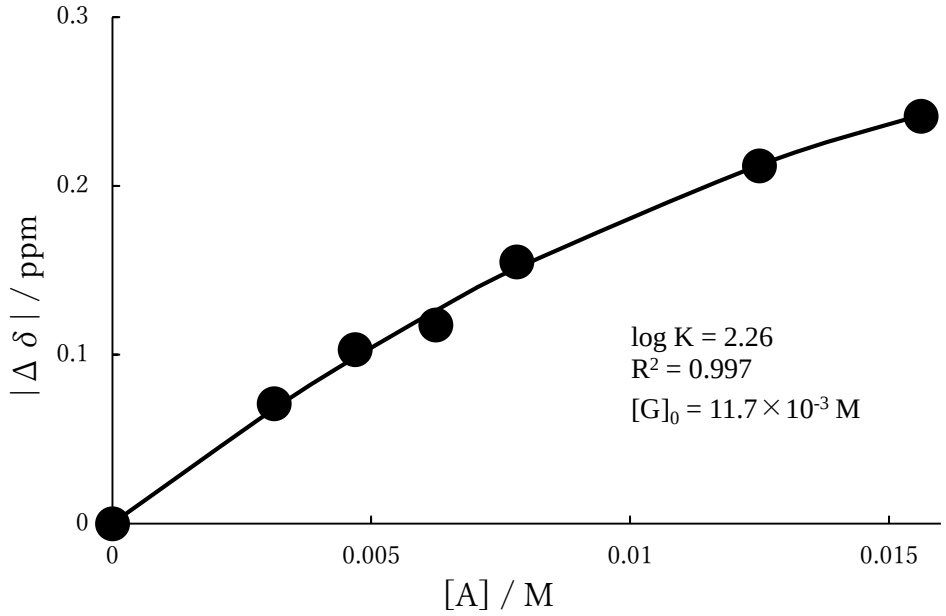


Figure S39. ^{31}P-NMR titration of PPh_3O with **7**.

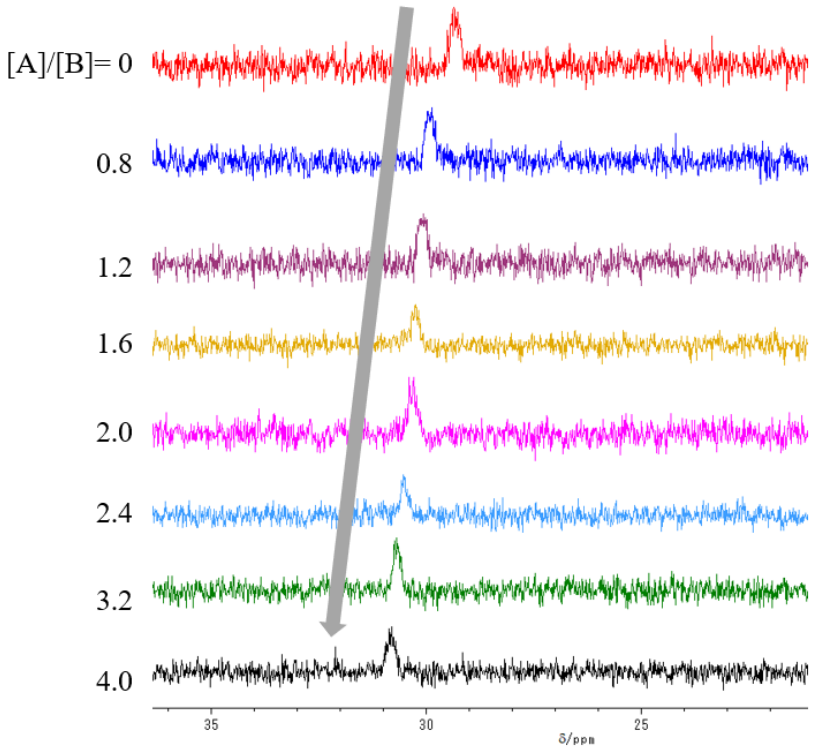


Figure S40. ^{31}P-NMR spectra of titration; PPh_3O with **8**.

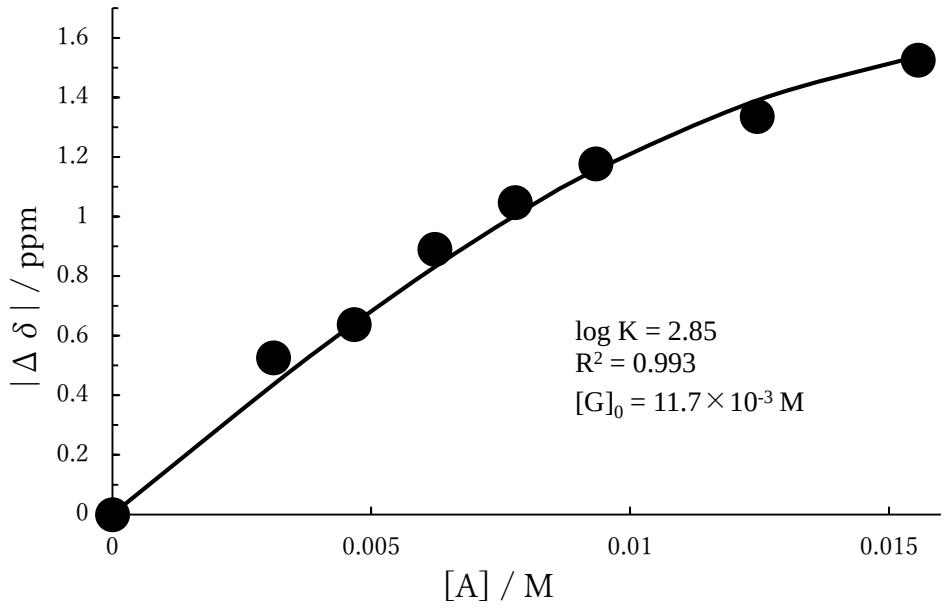


Figure S41. ^{31}P-NMR titration of PPh_3O with **8**.

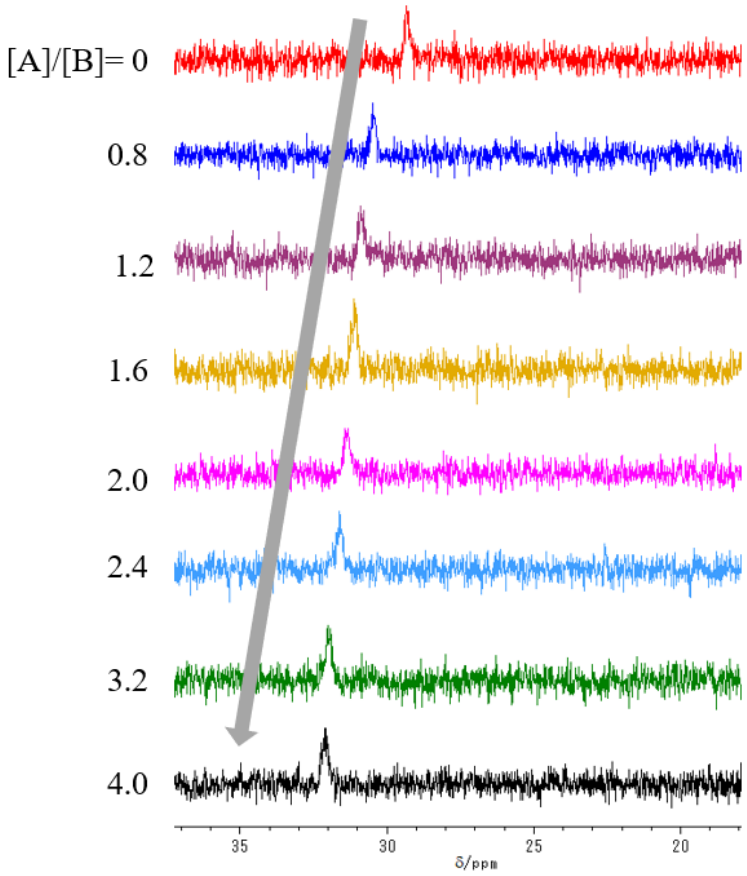


Figure S42. ^{31}P-NMR spectra of titration; PPh_3O with **10**.

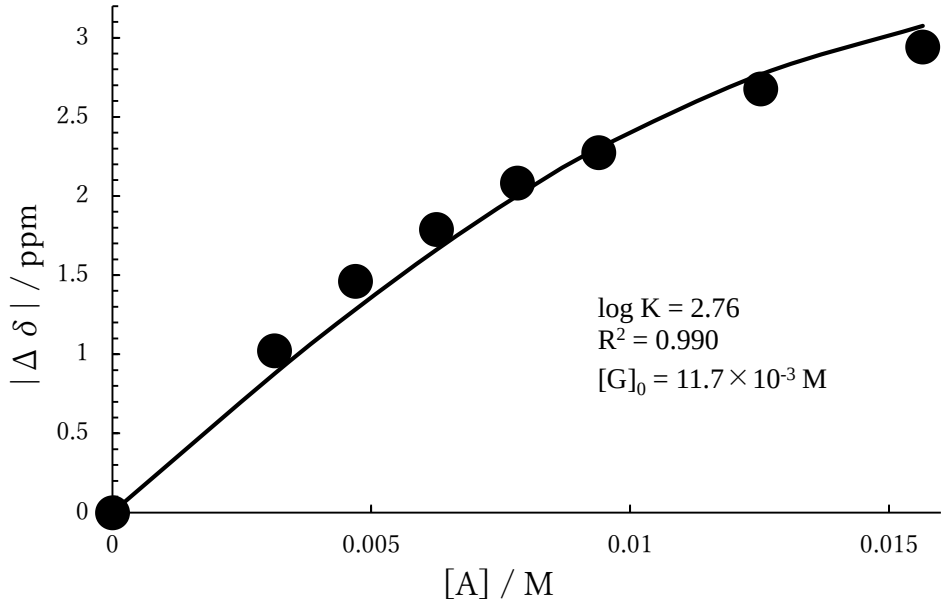


Figure S43. ^{31}P-NMR titration of PPh_3O with **10**.

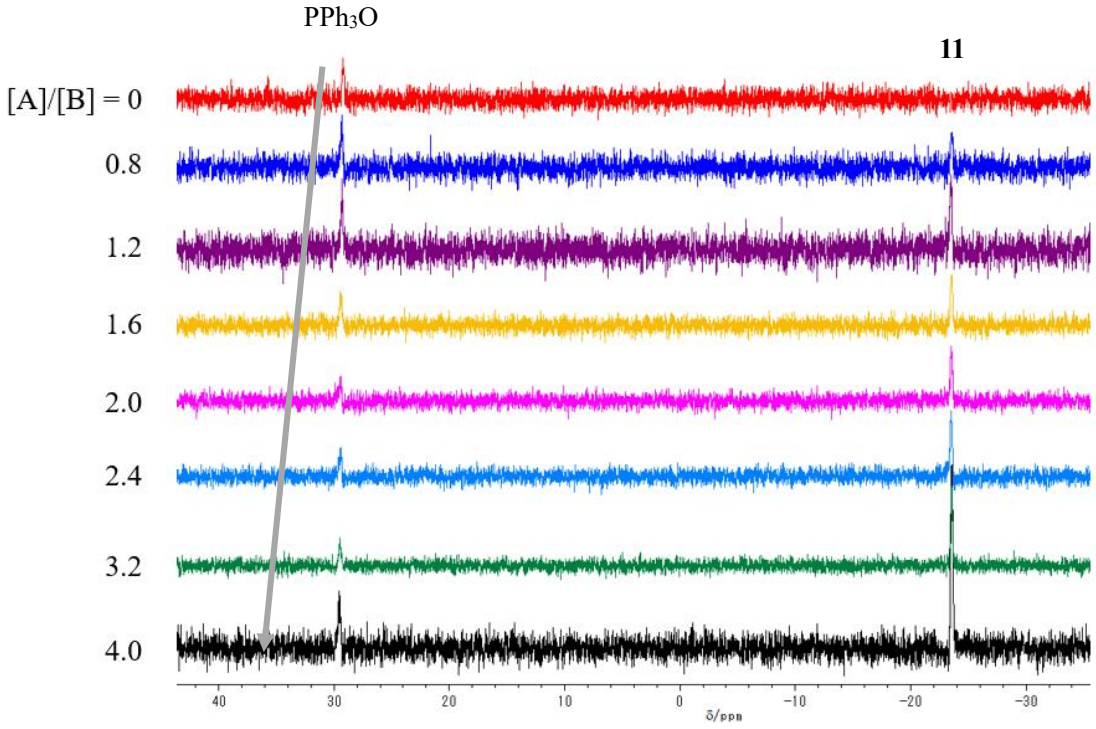


Figure S44. ^{31}P-NMR spectra of titration; PPh_3O with **11**.

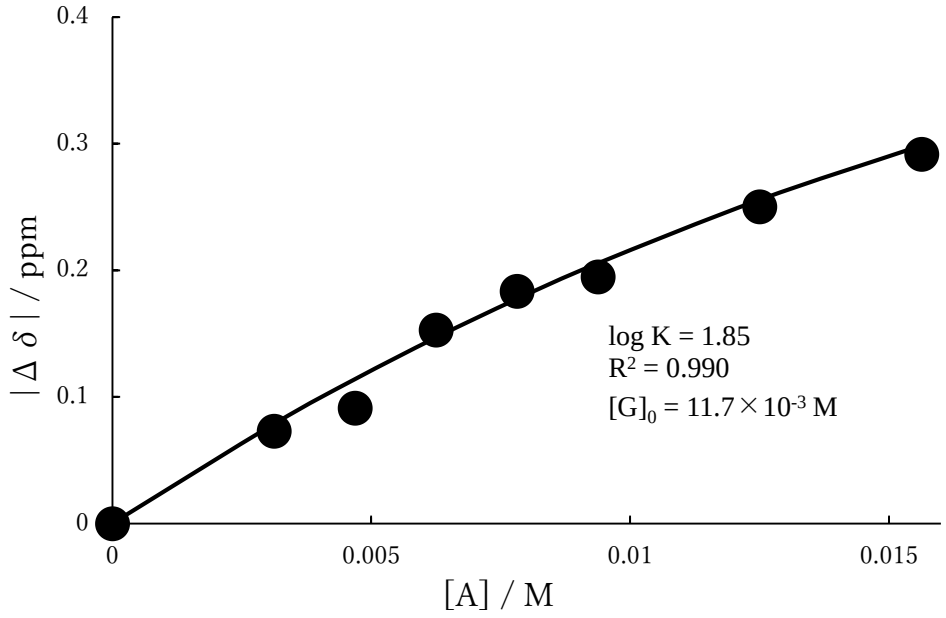


Figure S45. ^{31}P-NMR titration of PPh_3O with **11**.

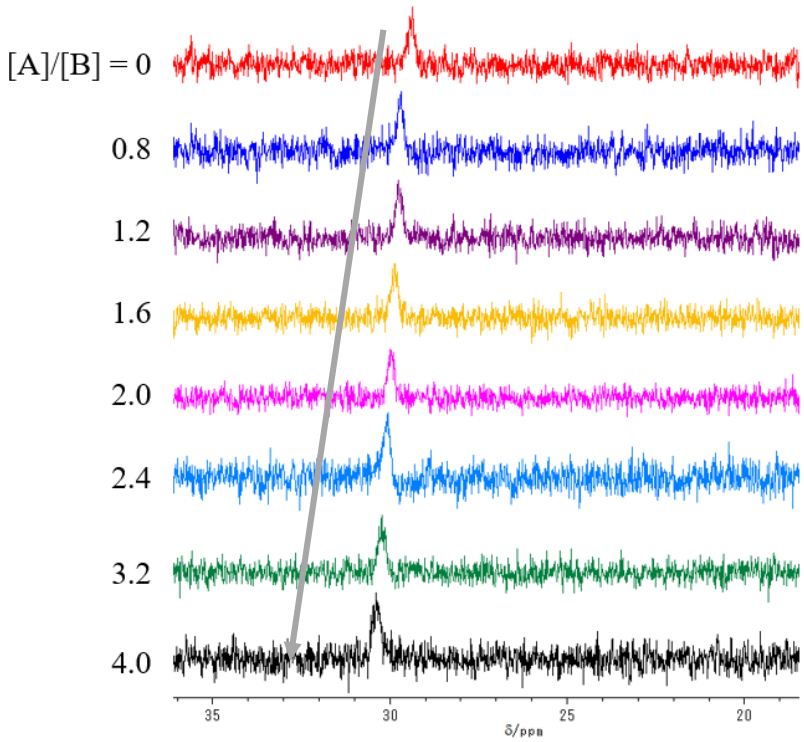


Figure S46. ^{31}P-NMR spectra of titration; PPh_3O with **12**.

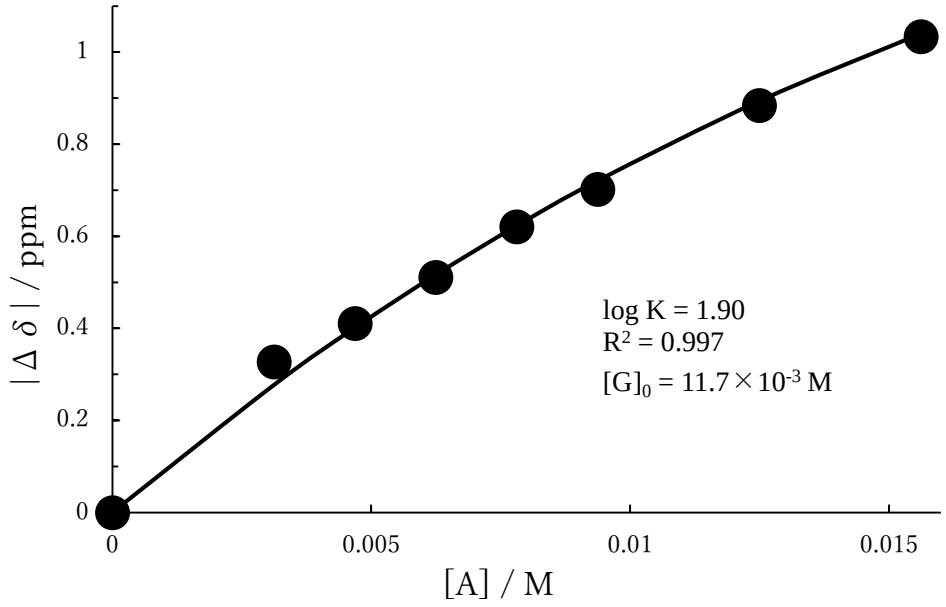


Figure S47. ^{31}P-NMR titration of PPh_3O with **12**.

6. Lewis acid-catalyzed bromination

A round bottom flask was charged with NBS (95.5 mg, 0.54 mmol), anisole (58 µL, 0.536 mmol) and tetrachlorocatecholates (27 µmol) in distilled $CDCl_3$ (8 mL). The mixture was stirred at room temperature for 24 h under N_2 atmosphere and the average NMR yields were estimated using dimethyl terephthalate as an internal standard by performing the experiment at least twice.

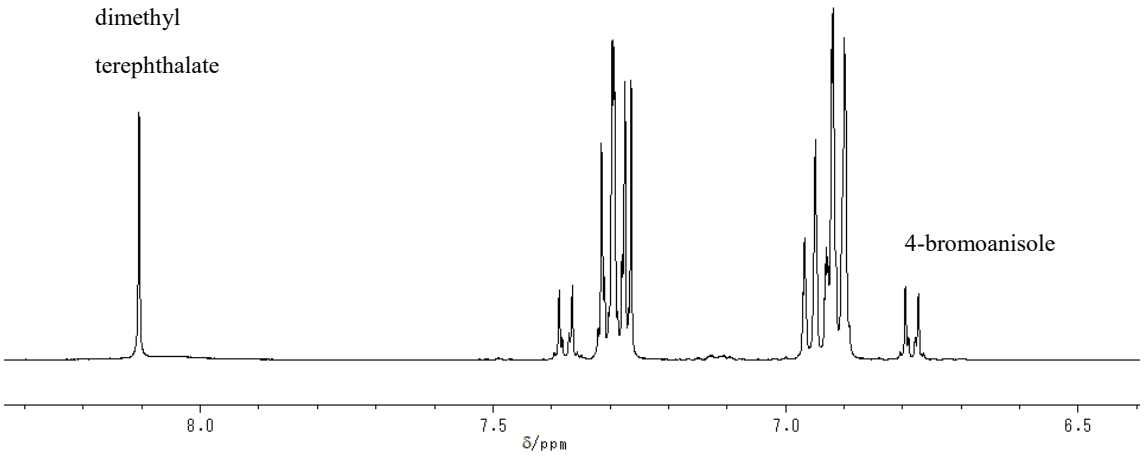


Figure S48. ^{1}H-NMR spectrum of the crude of the bromination reaction without catalyst.

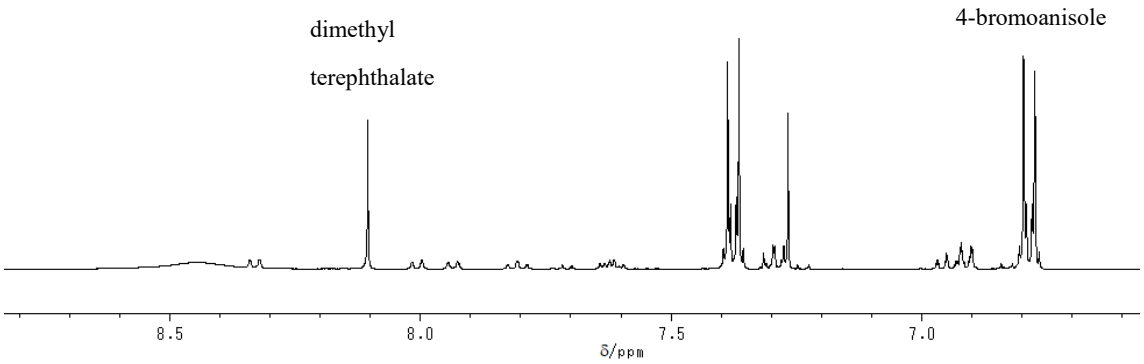


Figure S49. ^{1}H-NMR spectrum of the crude of the bromination reaction with **4** as a catalyst.

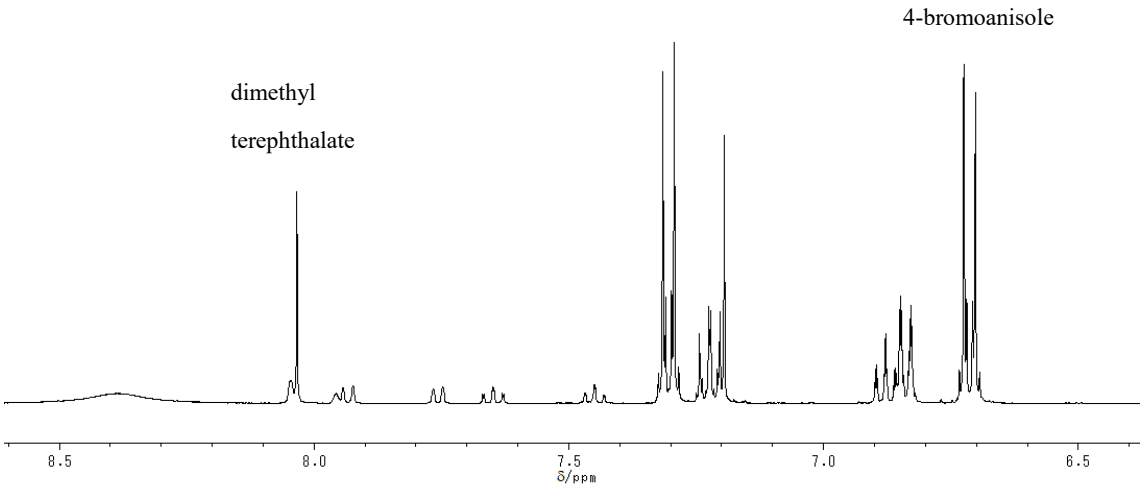


Figure S50. [1]H-NMR spectrum of the crude of the bromination reaction with **5** as a catalyst.

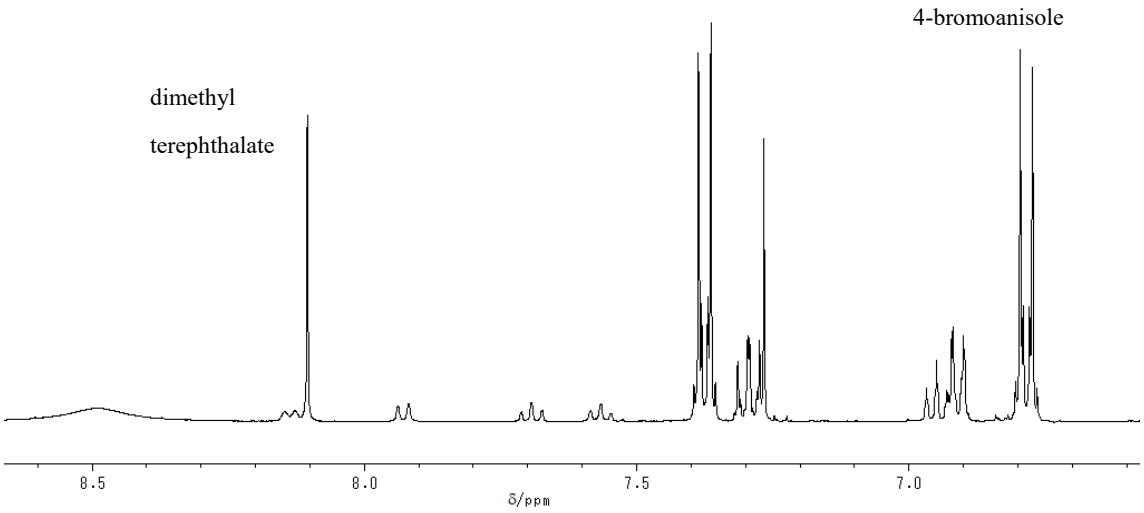


Figure S51. [1]H-NMR spectrum of the crude of the bromination reaction with **6** as a catalyst.

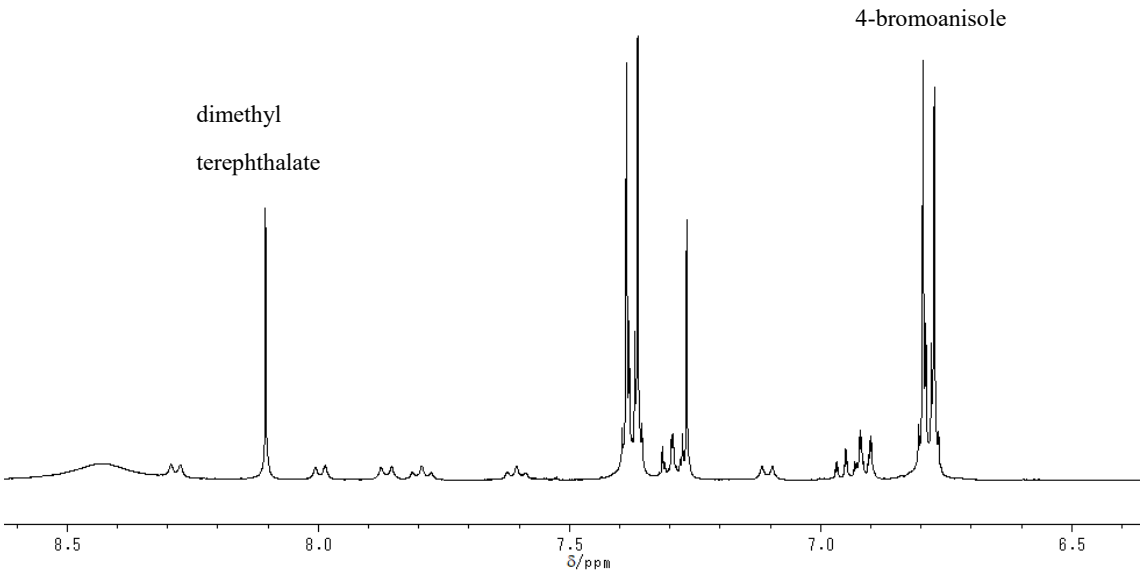


Figure S52. ^{1}H-NMR spectrum of the crude of the bromination reaction with **7** as a catalyst.

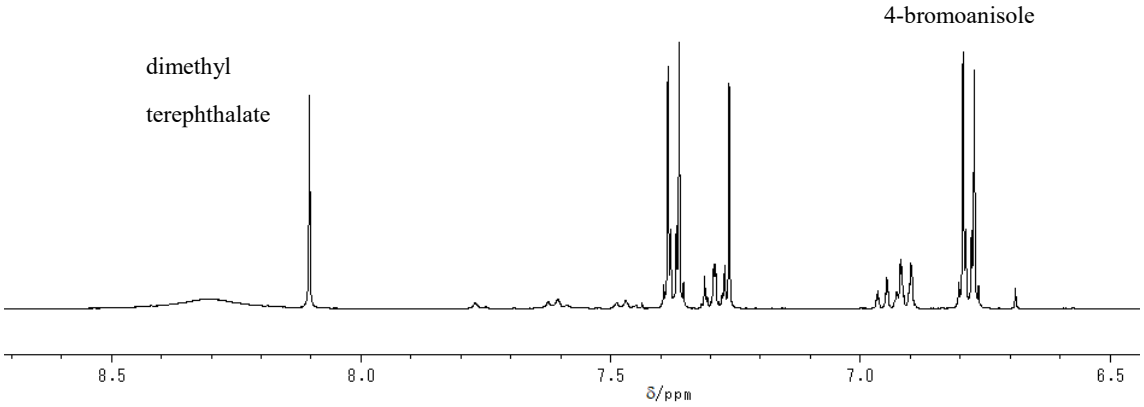


Figure S53. ^{1}H-NMR spectrum of the crude of the bromination reaction with **8** as a catalyst.

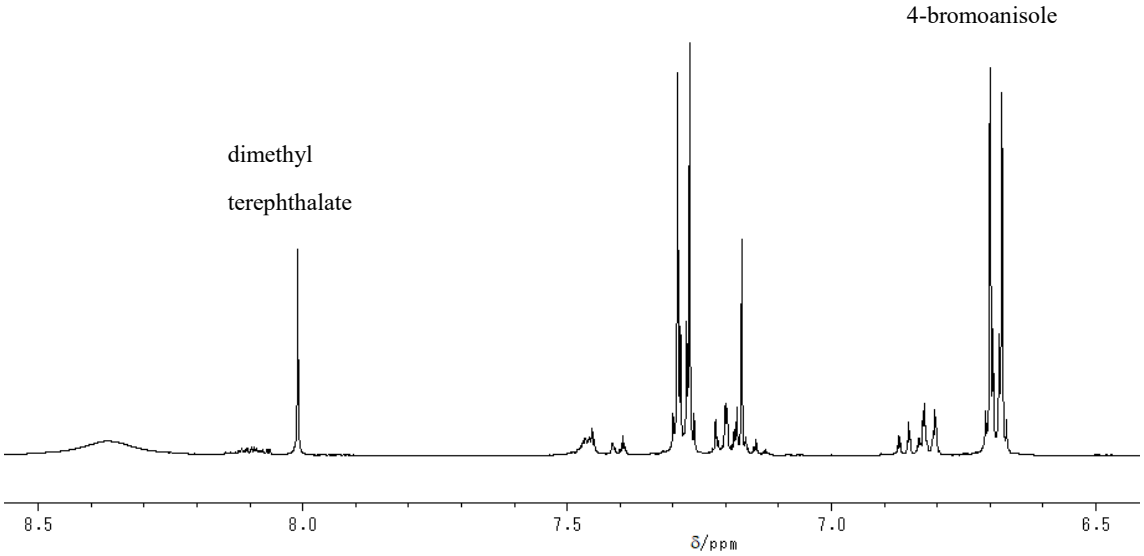


Figure S54. ^{1}H-NMR spectrum of the crude of the bromination reaction with **10** as a catalyst.

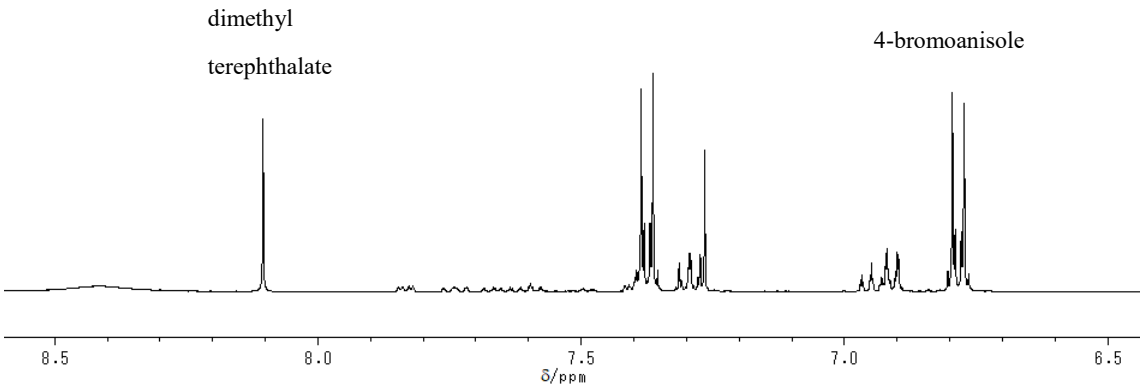


Figure S55. ^{1}H-NMR spectrum of the crude of the bromination reaction with **11** as a catalyst.

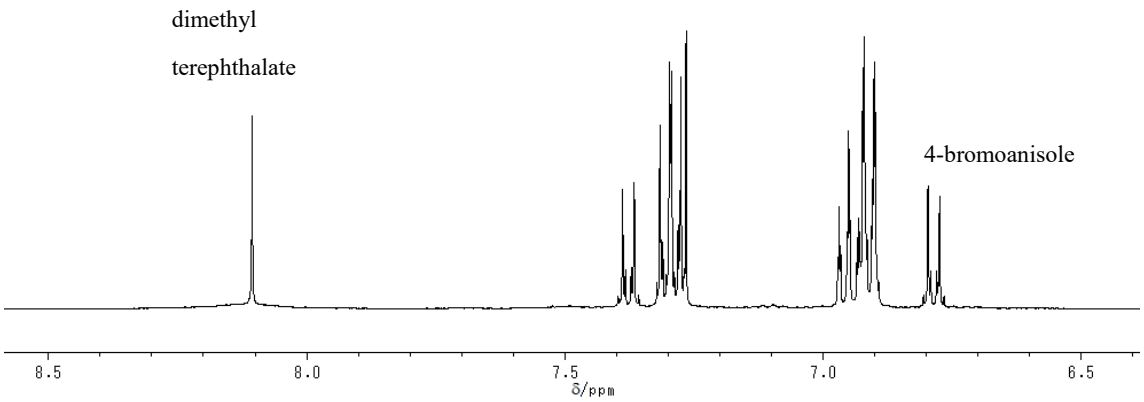


Figure S56. ^{1}H-NMR spectrum of the crude of the bromination reaction with **12** as a catalyst.

7. Computational calculations

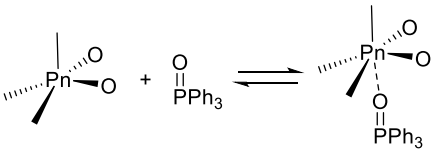
Table S18. Results of DFT and TD-DFT calculations[a,b]

	HOMO [eV]	LUMO [eV]	E[c] [eV]	f[d]		HOMO [eV]	LUMO [eV]	E[c] [eV]	f[d]
1	-5.72	-1.88	3.12	0.0068	**1'**	-6.22	-0.86	4.63	0.1088
2	-6.45	-2.99	2.80	0.0058	**2'**	-7.59	-2.42	4.42	0.0055
3	-5.52	-1.50	3.27	0.0125	**3'**	-5.68	-0.67	4.35	0.0127
4	-5.91	-2.31	2.93	0.0134	**4'**	-6.21	-1.39	4.29	0.0753
5	-6.15	-2.66	2.83	0.0108	**5'**	-6.52	-1.78	4.13	0.0004
6	-6.10	-2.64	2.80	0.0154	**6'**	-6.46	-1.72	4.11	0.0473
7	-5.84	-2.21	2.98	0.0132	**7'**	-6.10	-1.32	4.21	0.0564
8	-5.97	-2.51	2.84	0.0206	**8'**	-5.68	-1.63	3.62	0.1871
9	-5.86	-1.77	3.42	0.0117	**9'**	-5.99	-0.95	4.30	0.1240
10	-5.67	-1.98	2.92	0.0048	**10'**	-6.34	-0.93	4.67	0.1082
11	-6.17	-2.28	3.25	0.0301	**11'**	-6.20	-1.37	4.22	0.0587
12	-5.76	-2.34	2.76	0.0070	**12'**	-6.19	-1.44	4.17	0.0643

[a] The full geometries were optimized based on B3LYP/def2svp, and the single-point calculations were conducted based on B3LYP/def2tzvp.

[b] **2'**: tris(bis(3,5-trifluoromethyl)phenyl)arsine, **3'**: tri(*p*-anisyl)arsine.

[c] Transition energies and [d] oscillator strengths for HOMO-LUMO transitions.



	Stabilization energy [kcal/mol]
1	24.5
4	24.3
5	26.3
6	27.1
7	23.7
8	26.1
9	20.2
10	31.7
11	21.8
12	30.1

Figure S57. Stabilization energies for the complexation of the tetrachlorocatecholates with $O=PPh_3$. The full geometries were optimized based on B3LYP-D3BJ/def2svp, and the single point calculations were conducted based on B3LYP-D3BJ/def2tzvp. The substituents around the Pn atoms are omitted in the scheme for clarity.

Table S19. Activation energies of the transition states in the hydrolyses in tetrachlorocatecholates of Pn compounds, given in kcal/mol.[1]

Pn compounds	Label	TS1	TS2	TS3
Triphenylarsine	**1**	14.7	2.0	–
9-Phenyl-9-arsafluorene	**4**	19.1	3.9	1.8
Triphenylstibine	**10**	14.8	0.4	13.4
9-Phenyl-9-stibafluorene	**12**	15.3	3.3	17.8

[1] the activation energy (in kcal/mol) of a TS is measured from its reactant species at each elementary step. The activation energy values for the As(V) compounds were obtained at the dispersion-corrected B3LYP/SDD + 6-31G** //B3LYP/6-31G** level, and those for the Sb(V) compounds were at the dispersion corrected B3LYP/SDD + 6-31G** level.

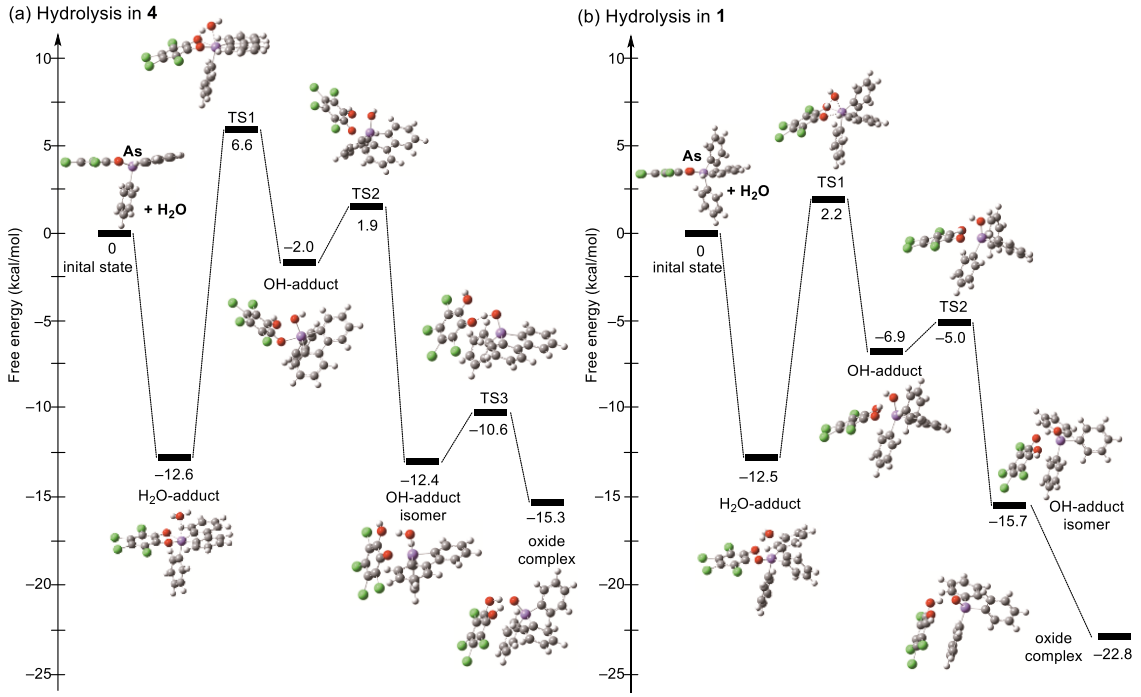


Figure S58. Free energy profiles of hydrolysis reactions between an As(V) compound and water molecule at the B3LYP-D3/SDD+6-31G**//B3LYP-D3/6-31G** level: hydrolysis in (a) **4** and (b) **1**. Their optimized geometries were obtained at the B3LYP-D3/6-31G** level, whose energies are shown.

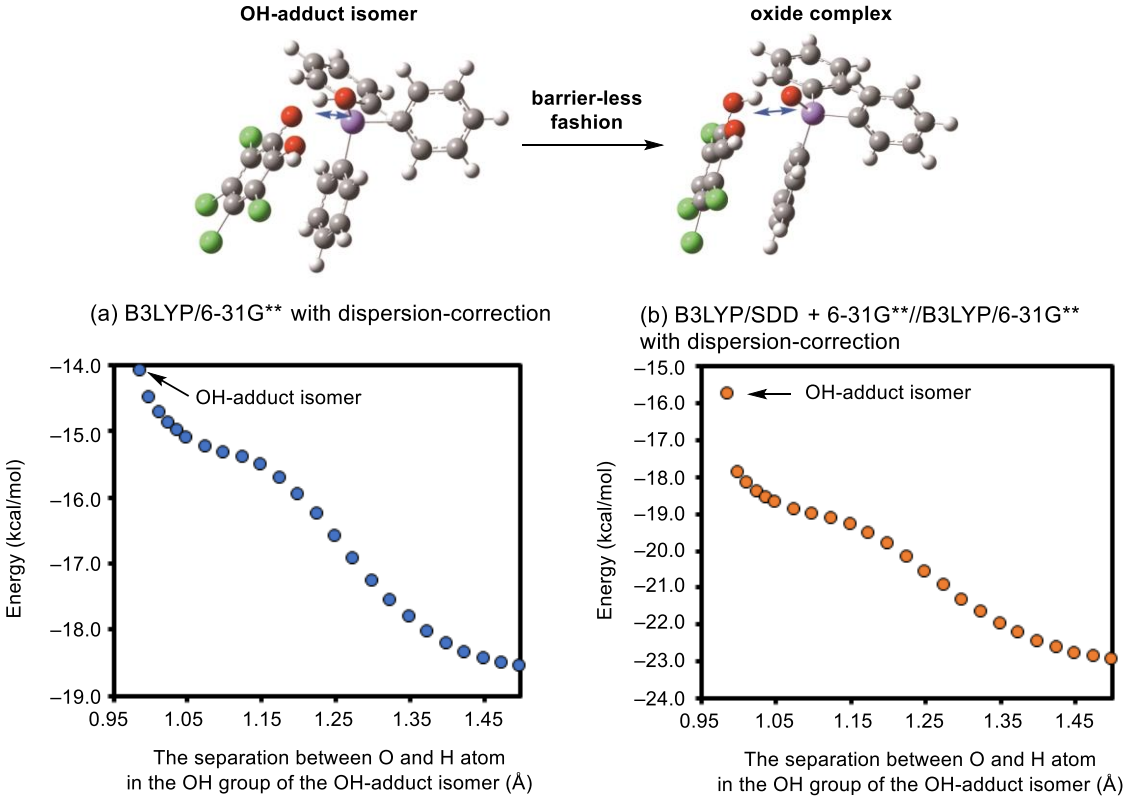


Figure S59. (a) The minimum-energy path analysis of hydrolysis of **1** at the dispersion-corrected B3LYP/6-31G** level, confirming that the formation of the oxide complex from the OH-adduct isomer proceeds in a barrier-less fashion. In the analysis, the separation between O and H atoms in the attached OH group in the OH-adduct isomer (the blue arrow) is kept to a certain value from 0.99 to 1.50 Å, but other parameters are fully relaxed. The energy changes by changing the OH separation in the interval of 0.0125 or 0.025 Å are displayed as a function of the OH separation. The same analysis was done at the dispersion-corrected B3LYP/SDD + 6-31G**//B3LYP/6-31G** level, whose graph is given in (b).

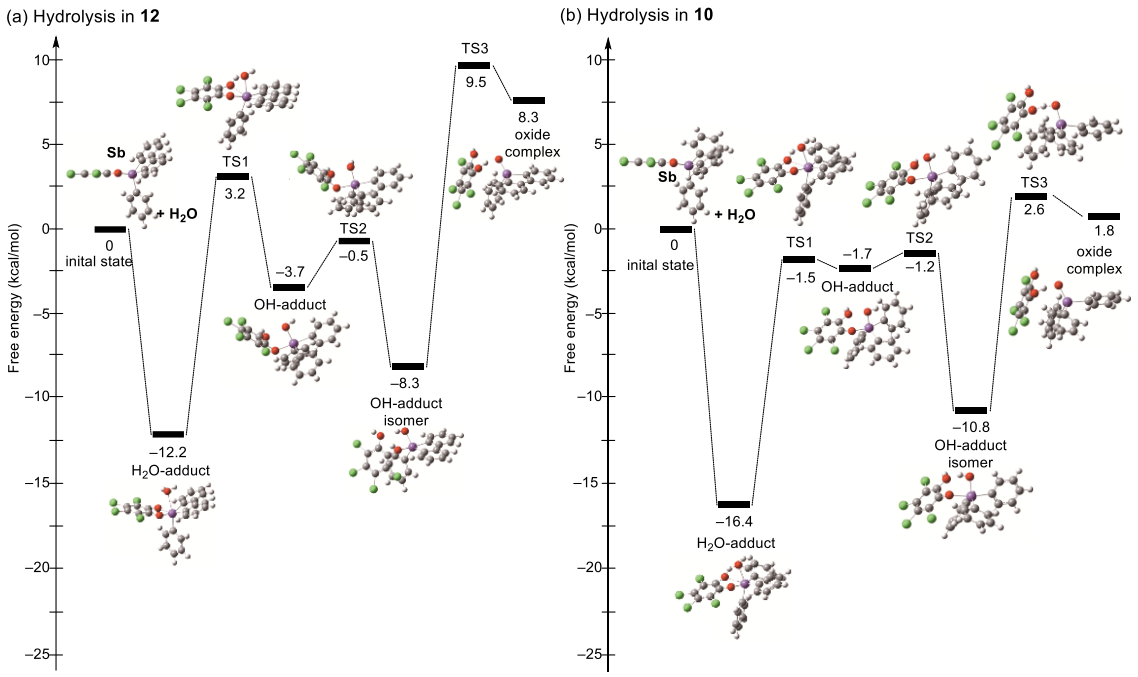


Figure S60. Free energy profiles of hydrolysis reactions between an As(V) compound and water molecule at the B3LYP-D3/SDD+6-31G**: hydrolysis in (a) **12** and (b) **10**. Their optimized geometries were obtained at the B3LYP-D3/6-31G** level, whose energies are shown.

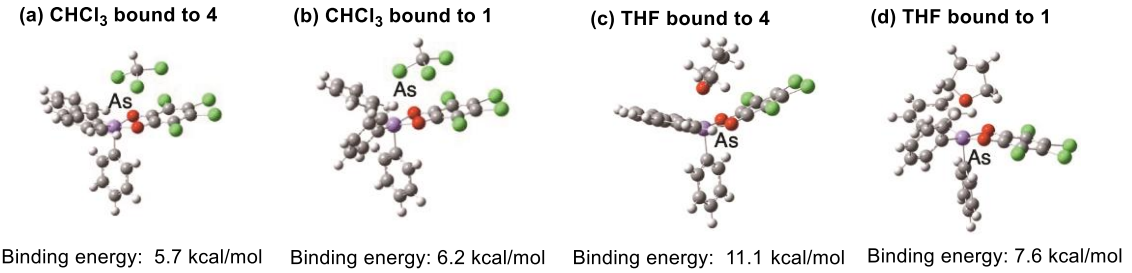


Figure S61. Optimized structures for $CHCl_3$ bound to **4** and **1** given in (a) and (b), respectively, obtained from dispersion-corrected B3LYP-D3/6-31G** level. Basis-set superposition error (BSSE) corrected binding energies are given in kcal/mol. Similarly, optimized structures for $CHCl_3$ bound to **4** and **1** given in (c) and (d), respectively, were obtained to compute their binding energies.

Table S20. τ_5 values of **1**-**12** estimated for the crystal and optimized structures.

	Crystal	Optimized by DFT[1]
1	0.76	0.77
2	0.23	0.76
3	0.53	0.77
4	0.10	0.32
5	0.05	0.32
6	0.17	0.34
7	0.07	0.39
8	0.07	0.38
9	0.91	0.88
10	0.66	0.73
11	0.02	0.10
12	0.12	0.48

[1] Optimized by DFT calculations (B3LYP/def2svp)

Cartesian coordinates in the structures optimized by DFT calculations

A. Optimized by B3LYP/def2svp

1 (S_0): E = -5149.124182 hartree

Atom	X	Y	Z
As	1.255059	-0.07723	-0.00324
Cl	-5.12866	2.135583	-0.14696
Cl	-2.18481	3.35402	-0.20227
Cl	-2.94273	-2.89462	0.002713
Cl	-5.50524	-1.0021	-0.04376
O	-0.36776	-1.29594	-0.11252
O	-0.06584	1.213936	-0.18292
C	2.599709	1.388546	-0.08385
C	-1.34711	0.783664	-0.15626
C	1.627346	-0.79737	1.786176
C	-1.49709	-0.6178	-0.11685
C	-3.91064	-0.31305	-0.08597
C	-2.78604	-1.16488	-0.07137
C	2.271395	2.748691	0.028197
H	1.229747	3.049805	0.132941
C	-3.74639	1.082483	-0.12963
C	-2.4465	1.635306	-0.15995
C	3.948828	1.021609	-0.22773
H	4.228869	-0.03149	-0.31972
C	1.902493	-1.12392	-1.52176
C	1.956407	-2.52382	-1.46039
H	1.655098	-3.05199	-0.55488
C	1.026103	-1.99012	2.226771
H	0.316362	-2.50796	1.583
C	2.492327	-0.09927	2.644291
H	2.953362	0.836226	2.32772
C	2.263549	-0.45632	-2.69935
H	2.221967	0.633826	-2.75395
C	3.279662	3.719656	-0.00439
H	3.011068	4.776001	0.079014

C	1.315306	-2.48546	3.500695
H	0.847363	-3.41532	3.833397
C	2.183388	-1.79283	4.349801
H	2.399965	-2.18113	5.348298
C	4.618691	3.346728	-0.14401
H	5.40194	4.108786	-0.169
C	4.952882	1.993093	-0.25447
H	5.9975	1.69108	-0.36576
C	2.764461	-0.59658	3.922149
H	3.433364	-0.04143	4.5844
C	2.680592	-1.19002	-3.81458
H	2.950972	-0.66733	-4.73541
C	2.397354	-3.24792	-2.57037
H	2.45178	-4.33807	-2.51687
C	2.754707	-2.58375	-3.74876
H	3.088397	-3.15535	-4.61847

2 (S_0): E = -7169.832431 hartree

Atom	X	Y	Z
As	-0.07699	-0.07766	0.106226
Cl	-1.96065	-3.99342	2.276192
Cl	-4.92612	1.17922	0.252412
Cl	-6.61037	-1.18266	1.571998
Cl	-5.12535	-3.77933	2.588309
O	-0.77454	-1.52764	1.008184
F	-2.06474	1.876193	-5.78986
O	-1.95894	0.550713	0.209783
F	4.620525	-4.634	1.168311
F	3.177003	-4.20646	2.72513
F	-2.79047	2.52997	-3.85211
F	-3.50224	0.674871	-4.70743
F	-0.62336	6.226789	1.484769
F	2.781607	-1.73498	-4.18895
F	2.511223	-5.01128	0.832671
F	6.313969	-0.57805	-0.85342

F	1.127816	-2.70149	-5.19595
F	5.010878	1.122747	-1.19946
F	0.705903	5.915379	-0.19221
F	5.833314	0.767199	0.769995
F	-1.33444	5.200984	-0.29045
F	2.78934	3.933956	4.340793
C	-2.76735	-0.36596	0.729424
C	-2.12148	-1.52906	1.179993
C	1.723643	-0.9205	0.31156
C	-2.82647	-2.58538	1.747479
C	0.355453	1.626712	0.974034
C	1.913844	-2.22859	0.77276
H	1.057829	-2.83812	1.060124
F	1.947748	-0.86713	-5.99501
C	-4.2287	-2.47733	1.874561
C	-0.19682	-0.03553	-1.85835
C	3.209242	-2.75813	0.864984
C	-4.88798	-1.31846	1.422621
C	-0.13316	2.835428	0.46134
H	-0.74642	2.859703	-0.43895
C	2.842352	-0.15524	-0.05397
H	2.726204	0.865812	-0.42462
C	-1.29026	0.707263	-3.88954
C	-4.15771	-0.26043	0.841169
C	-1.22789	0.673519	-2.49313
H	-1.98708	1.182551	-1.90051
C	-0.34841	0.022675	-4.66049
H	-0.39553	0.06363	-5.74965
F	2.987162	1.777863	4.189647
C	4.129474	-0.68966	0.035576
C	0.740669	-0.73496	-2.63033
H	1.544001	-1.3025	-2.16301
C	1.104214	1.614938	2.154186
H	1.493164	0.681204	2.564143
C	3.385109	-4.16363	1.398431
C	4.317827	-1.9975	0.495517

H	5.320569	-2.42153	0.555755
C	0.163428	4.032202	1.117104
C	0.658084	-0.7088	-4.0254
F	1.2662	2.643262	5.173634
C	-2.41992	1.456249	-4.56532
C	5.329863	0.159873	-0.31833
C	0.905521	4.026741	2.303112
H	1.122388	4.96306	2.819184
C	1.365202	2.816468	2.823789
C	1.639397	-1.50689	-4.85679
C	-0.28184	5.352659	0.526153
C	2.111146	2.794207	4.140513

3 (S_0): *E* = -5492.442964 hartree

Atom	X	Y	Z
As	0.677334	-0.03999	0.073684
Cl	-2.32097	0.553544	-3.70851
Cl	-5.38206	0.71502	-2.83905
Cl	-6.1318	0.555022	0.229414
Cl	-3.82092	0.237621	2.39998
O	-0.47605	0.296928	-1.34479
O	-1.07658	0.181367	1.11412
O	1.161898	-5.79386	2.11359
O	2.548513	4.486094	3.72286
O	5.386451	-0.20441	-3.89575
C	2.168034	-0.04987	-1.23336
C	-1.7948	0.366586	-1.06269
C	-2.11062	0.301031	0.311673
C	1.984768	-0.112	-2.62813
H	0.977533	-0.11442	-3.04332
C	0.794469	-1.86643	0.760957
C	1.3168	1.388134	1.231824
C	-4.4683	0.481909	-0.27069
C	2.346588	3.580557	1.467604
H	2.808305	4.447513	0.99525

C	-3.45586	0.348198	0.702667
C	-4.1386	0.550632	-1.63503
C	0.004291	-2.30014	1.837987
H	-0.7171	-1.61757	2.285355
C	3.07849	-0.16101	-3.48763
H	2.942182	-0.20428	-4.57025
C	1.926404	2.512529	0.667195
H	2.080935	2.573155	-0.4122
C	-2.78405	0.486278	-2.03278
C	1.675497	-2.78639	0.15873
H	2.288349	-2.48997	-0.69243
C	0.106002	-3.60556	2.323405
H	-0.52256	-3.9047	3.162172
C	1.120107	1.341907	2.624682
H	0.620658	0.48854	3.08422
C	3.479907	-0.04022	-0.73892
H	3.662999	0.008092	0.338166
C	0.994718	-4.51276	1.722883
C	4.587331	-0.09426	-1.59175
H	5.589794	-0.08549	-1.16349
C	2.169756	3.518672	2.8585
C	1.55663	2.385569	3.42868
H	1.423194	2.359315	4.511903
C	1.773332	-4.08945	0.630242
H	2.448765	-4.809	0.163431
C	4.389958	-0.15376	-2.98102
C	0.402896	-6.30044	3.19264
H	0.606492	-5.75161	4.129088
H	0.705302	-7.34813	3.320173
H	-0.68064	-6.26241	2.983518
C	3.146815	5.666178	3.230001
H	3.356299	6.297454	4.1036
H	2.472668	6.21219	2.546459
H	4.095314	5.456078	2.704097
C	6.728984	-0.20414	-3.46258
H	6.980684	0.715402	-2.90413

H	7.349192	-0.25114	-4.36759
H	6.956335	-1.07924	-2.82754

4 (S_0): E = -5147.942239 hartree

Atom	X	Y	Z
As	-1.16029	-0.03864	0.034299
Cl	2.788254	-3.00975	-0.37689
Cl	5.470349	-1.28586	-0.49958
Cl	5.293	1.870304	-0.45242
Cl	2.438557	3.276442	-0.28635
O	0.330246	-1.2577	-0.27288
O	0.184739	1.262983	-0.22143
C	-2.30226	-1.2436	-0.99838
C	-2.05369	-2.57592	-1.32777
C	-3.03622	-3.2971	-2.0167
C	-4.24247	-2.67971	-2.36569
C	-4.47879	-1.33954	-2.04407
C	-3.50262	-0.60154	-1.36046
C	-3.6018	0.837227	-0.9978
C	-4.67459	1.684501	-1.31054
C	-4.61618	3.037564	-0.96351
C	-3.49182	3.560001	-0.314
C	-2.41751	2.721457	0.008433
C	-2.48892	1.367009	-0.31876
C	-1.30044	-0.40455	1.942525
C	-2.15298	0.368915	2.744615
C	-2.26347	0.093983	4.110728
C	-1.52681	-0.94874	4.679352
C	-0.67744	-1.71932	3.879619
C	-0.56076	-1.4527	2.512972
C	1.507087	-0.63696	-0.31327
C	1.432696	0.770236	-0.28347
C	2.588951	1.546848	-0.32638
C	3.847396	0.908896	-0.39722
C	3.926043	-0.49478	-0.42037

C	2.748948	-1.27185	-0.37245
H	-1.10124	-3.035	-1.06056
H	-2.85696	-4.34087	-2.28568
H	-5.00704	-3.2464	-2.90318
H	-5.42275	-0.87373	-2.33486
H	-5.55259	1.299844	-1.83392
H	-5.45286	3.69445	-1.21457
H	-3.44756	4.623437	-0.06631
H	-1.52604	3.121664	0.495507
H	-2.73256	1.185747	2.311744
H	-2.92796	0.700263	4.731339
H	-1.61382	-1.16064	5.748063
H	-0.09849	-2.53473	4.320305
H	0.102844	-2.05275	1.889455

5 (S_0): *E* = -5821.512401 hartree

Atom	X	Y	Z
As	-0.50914	-1.09261	0.359392
Cl	3.464177	0.936059	2.514784
Cl	2.856234	-1.77638	-3.13441
Cl	5.665047	-0.53087	-2.29032
Cl	5.972736	0.828562	0.545993
F	-5.23967	2.120362	-1.38252
O	0.781784	-1.47396	-0.95614
O	1.033636	-0.39418	1.311768
F	-4.13699	1.183059	-2.99011
F	-4.0931	3.339489	-2.75215
F	0.607118	4.183876	1.200162
F	-0.91001	5.406404	0.245692
F	-1.3015	4.494714	2.168298
C	4.318082	-0.46795	-1.19716
C	4.455428	0.135875	0.066121
C	3.080222	-1.02611	-1.58544
C	-1.21614	-1.76039	2.05271
C	3.357451	0.188265	0.950941

C	2.138743	-0.37189	0.564483
C	-2.27001	-2.6668	1.823495
C	-1.71972	-2.34952	-0.54083
C	2.003677	-0.97084	-0.70224
C	-2.54142	-2.99903	0.399455
C	-2.34811	0.790508	-0.90854
H	-2.77468	-0.08852	-1.39263
C	-0.81614	-1.40568	3.340974
H	0.024642	-0.72607	3.484623
C	-1.26043	0.670677	-0.03516
C	-2.88963	2.051306	-1.17913
C	-1.26688	3.070277	0.288473
C	-1.81462	-2.62955	-1.90448
H	-1.13791	-2.14786	-2.61313
C	-0.71719	1.814275	0.564693
H	0.138409	1.725526	1.234995
C	-2.77359	-3.5494	-2.3467
H	-2.85831	-3.77955	-3.41144
C	-1.50094	-1.95009	4.43398
H	-1.20023	-1.68613	5.450637
C	-2.56395	-2.8354	4.223718
H	-3.09606	-3.25751	5.079929
C	-2.34979	3.194657	-0.58522
H	-2.76158	4.178778	-0.81221
C	-2.94914	-3.19703	2.928857
H	-3.77465	-3.89778	2.787933
C	-3.61526	-4.18012	-1.42345
H	-4.3626	-4.8974	-1.77171
C	-3.50126	-3.91419	-0.05547
H	-4.15556	-4.43053	0.650102
C	-4.09391	2.17446	-2.08525
C	-0.70965	4.297339	0.97626

6 (S_0): *E* = -5643.695845 hartree

Atom	X	Y	Z

As	0.937338	-0.59531	0.158105
Cl	-5.61586	-1.02752	-1.33605
Cl	-2.84496	-1.87317	-2.6639
Cl	-2.855	0.858138	3.01013
Cl	-5.61905	0.340539	1.51172
F	0.922468	0.782061	-2.67226
O	-0.48813	-1.19922	-0.89575
F	1.862718	5.215742	-1.48132
F	1.323053	3.337448	-3.37822
F	2.006087	4.505236	1.141562
F	1.606044	1.960616	1.877001
O	-0.4927	-0.09788	1.372041
C	-4.12187	-0.7365	-0.50087
C	2.167363	-1.64798	-0.95954
C	4.166109	-3.15769	-2.1677
H	4.953817	-3.746	-2.64502
C	-1.70888	-0.87075	-0.42841
C	-2.90227	-1.114	-1.10446
C	3.164436	-1.82248	1.271092
C	4.09128	-2.23615	2.238131
H	4.981709	-2.79703	1.947241
C	-4.122	-0.1255	0.766414
C	1.798899	-0.80931	3.03663
H	0.902132	-0.26306	3.328479
C	1.271571	1.264538	-0.37205
C	2.065248	-1.95484	-2.31657
H	1.203866	-1.61833	-2.89304
C	1.196324	1.662726	-1.71194
C	3.239816	-2.12468	-0.18206
C	2.035735	-1.09322	1.691332
C	3.074992	-2.71254	-2.92175
H	3.005153	-2.96116	-3.98348
C	4.250333	-2.87293	-0.8018
H	5.097746	-3.24759	-0.22393
C	-1.70232	-0.25578	0.838329
C	3.870111	-1.94225	3.586814

H	4.594699	-2.27433	4.334631
C	2.728147	-1.24016	3.98939
H	2.558972	-1.02901	5.047868
C	1.670725	3.954819	-1.12745
C	1.533755	2.255865	0.583162
C	1.398636	2.989572	-2.09947
C	-2.90645	0.115344	1.441845
C	1.74465	3.587686	0.218664

7 (S_0): E = -5262.382315 hartree

Atom	X	Y	Z
As	1.053519	-0.39719	0.106534
Cl	-2.85593	1.024185	2.826852
Cl	-5.46124	-1.12436	-1.49704
Cl	-5.57416	0.345866	1.299884
Cl	-2.63435	-1.90674	-2.74153
O	-0.34156	-1.10544	-0.94495
O	-0.43725	0.061713	1.295772
O	2.273554	5.349869	-1.54138
C	2.30915	-1.46639	-0.96695
C	3.217229	-1.68519	1.293754
C	2.080385	-0.94588	1.67568
C	1.407606	1.439417	-0.40506
C	0.749989	2.498097	0.237034
H	0.022227	2.287886	1.021383
C	-4.04616	-0.10111	0.604325
C	3.337732	-1.98362	-0.15795
C	-1.62381	-0.16181	0.740685
C	-1.57882	-0.81028	-0.51055
C	-2.85323	0.201151	1.294988
C	-3.99621	-0.75294	-0.64026
C	1.949481	4.107013	-1.12626
C	4.113703	-2.09864	2.288914
H	5.007329	-2.669	2.026742
C	1.815437	-0.64319	3.011107

H	0.91082	-0.09445	3.27533
C	1.01379	3.823154	-0.11729
H	0.48305	4.6228	0.399311
C	2.25711	-1.7421	-2.33353
H	1.427091	-1.36938	-2.93745
C	4.349148	-2.75357	-0.75049
H	5.161171	-3.16458	-0.14672
C	-2.75019	-1.10895	-1.20323
C	2.613152	3.045696	-1.76997
H	3.336648	3.28383	-2.55204
C	2.345165	1.729916	-1.41413
H	2.872682	0.925669	-1.92912
C	1.645713	6.47014	-0.95162
H	1.855381	6.533553	0.130767
H	0.552239	6.453286	-1.10455
H	2.061975	7.35643	-1.44814
C	3.861498	-1.78804	3.62876
H	4.563486	-2.11866	4.398533
C	2.717555	-1.06931	3.993261
H	2.523816	-0.84402	5.044789
C	4.312136	-3.0115	-2.12397
H	5.100042	-3.61637	-2.57995
C	3.268577	-2.51689	-2.91481
H	3.237649	-2.74221	-3.98371

8 (S_0): *E* = -5789.336376 hartree

Atom	X	Y	Z
As	-1.0547	-0.07121	0.140547
Cl	5.349209	1.968209	-0.33372
Cl	2.489064	3.301613	0.096828
S	-4.36933	-1.34134	-2.39114
Cl	5.559329	-1.15721	-0.75536
S	-4.69282	2.126364	-0.94295
Cl	2.904287	-2.92485	-0.74037
O	0.259491	1.262799	0.016671

O	0.430944	-1.2355	-0.33897
C	-3.33865	-0.41683	-1.35716
C	-2.41735	1.350386	0.004396
C	-3.47016	0.912345	-0.77928
C	1.511946	0.79568	-0.14938
C	-2.16857	-1.10247	-1.07734
C	4.010592	-0.4053	-0.52718
C	2.655902	1.590971	-0.14641
C	3.917615	0.98489	-0.33739
C	1.599421	-0.59724	-0.34659
C	-2.08842	-2.37618	-1.70363
H	-1.23437	-3.04743	-1.61674
C	-1.18469	-0.70014	1.97675
C	-2.58631	2.684737	0.465836
H	-1.85731	3.225719	1.070165
C	-3.21319	-2.64348	-2.44667
H	-3.43563	-3.5297	-3.03963
C	2.845453	-1.20125	-0.52711
C	-2.01639	-0.03207	2.887736
H	-2.58629	0.845452	2.578044
C	-3.77641	3.229361	0.040305
H	-4.16962	4.226376	0.235284
C	-0.45663	-1.82893	2.384944
H	0.191497	-2.34371	1.674807
C	-0.5657	-2.2822	3.702078
H	0.002765	-3.16039	4.018079
C	-1.3944	-1.61742	4.611134
H	-1.47499	-1.97529	5.64071
C	-2.11838	-0.49355	4.203122
H	-2.76595	0.030233	4.910574

9 (S_0): E = -3254.770857 hartree

Atom	X	Y	Z
Cl	-4.94837	2.154765	-0.00329
Cl	-1.98242	3.332298	-0.01196

Cl	-2.84095	-2.91436	-0.05435
Cl	-5.37012	-0.97602	-0.02596
O	-0.22232	-1.30346	-0.07972
O	0.108809	1.114985	-0.06083
C	2.633301	1.246413	-0.03007
C	-1.20252	0.741387	-0.05028
C	1.723772	-0.85796	1.635769
C	-1.36306	-0.65264	-0.06136
C	-3.76502	-0.31309	-0.03481
C	-2.65707	-1.18828	-0.05076
C	2.383873	2.623718	0.09024
H	1.361155	2.982806	0.198492
C	-3.58202	1.082318	-0.02417
C	-2.27398	1.620133	-0.0291
C	3.967204	0.820857	-0.17563
H	4.194697	-0.24382	-0.27648
C	1.828614	-0.93969	-1.5347
C	2.13391	-2.30833	-1.57712
H	2.088726	-2.91459	-0.67163
C	1.354382	-2.18082	1.956506
H	0.777788	-2.76956	1.246191
C	2.394289	-0.09205	2.607759
H	2.678839	0.938297	2.39682
C	1.881055	-0.18096	-2.71402
H	1.654659	0.887689	-2.69136
C	3.439384	3.544174	0.066544
H	3.222988	4.611859	0.157797
C	1.689158	-2.72714	3.196542
H	1.406646	-3.75849	3.421698
C	2.358677	-1.95754	4.152368
H	2.606513	-2.3852	5.127258
C	4.75748	3.106677	-0.07361
H	5.578923	3.827612	-0.09208
C	5.019343	1.737555	-0.19406
H	6.046727	1.381911	-0.30722
C	2.697699	-0.63519	3.858807

H	3.20588	-0.0181	4.603753
C	2.226063	-0.78826	-3.92423
H	2.252198	-0.19202	-4.83967
C	2.506254	-2.90329	-2.78487
H	2.757194	-3.96671	-2.80695
C	2.546296	-2.14803	-3.96101
H	2.827018	-2.6199	-4.90593
P	1.298473	-0.0865	0.007993

10 (S_0): *E* = -3153.808578 hartree

Atom	X	Y	Z
Sb	-1.23826	-0.10426	-6.8E-05
Cl	5.674598	-0.96571	-0.00019
Cl	3.097473	-2.83941	0.000533
Cl	2.379608	3.410441	-0.00249
Cl	5.312162	2.176728	-0.00172
O	0.249062	1.32228	-0.00176
O	0.552055	-1.27791	-0.00064
C	1.508833	0.852778	-0.0015
C	-1.77317	-1.09302	1.842993
C	1.663843	-0.55466	-0.00086
C	-1.77578	-1.09614	-1.8407
C	2.627523	1.68833	-0.00173
C	4.083915	-0.26526	-0.00068
C	-2.65107	1.555915	-0.00053
C	3.923862	1.130784	-0.00135
C	2.951955	-1.10505	-0.00039
C	-2.75259	-0.53788	-2.67773
H	-3.24447	0.400748	-2.41632
C	-2.74887	-0.53344	2.680429
H	-3.24123	0.404675	2.418084
C	-4.53174	3.641495	-0.00107
H	-5.26233	4.454506	-0.0013
C	-4.0279	1.272694	0.000621
H	-4.38839	0.239396	0.00176

C	-1.13083	-2.28886	-2.20572
H	-0.33921	-2.6969	-1.57641
C	-1.12758	-2.28505	2.209127
H	-0.33678	-2.69406	1.579405
C	-3.0963	-1.18249	-3.87094
H	-3.85433	-0.74214	-4.52367
C	-4.96455	2.311968	0.000353
H	-6.0329	2.080313	0.001261
C	-2.46891	-2.37902	-4.22786
H	-2.73924	-2.88086	-5.16048
C	-2.22146	2.892211	-0.00193
H	-1.15535	3.120931	-0.00277
C	-1.48699	-2.92786	-3.39691
H	-0.98523	-3.85675	-3.67979
C	-3.1637	3.927472	-0.0022
H	-2.82144	4.965674	-0.00329
C	-1.48199	-2.92206	3.401898
H	-0.97975	-3.85042	3.685659
C	-3.09083	-1.17606	3.875213
H	-3.84799	-0.73469	4.528267
C	-2.46281	-2.37191	4.233288
H	-2.73178	-2.8722	5.167126

11 (S_0): *E* = -3253.592690 hartree

Atom	X	Y	Z
C	-2.19005	-2.65765	-0.88425
C	-2.38781	-1.2793	-0.75268
C	-3.62827	-0.70512	-1.09151
C	-4.67846	-1.52007	-1.53081
C	-4.48154	-2.89893	-1.64687
C	-3.24199	-3.46559	-1.33159
C	-3.65827	0.767819	-0.9612
C	-2.44578	1.318134	-0.5058
C	-2.29705	2.705561	-0.40373
C	-3.37326	3.541476	-0.72531

C	-4.58743	2.992665	-1.15253
C	-4.73359	1.60808	-1.27569
C	-1.27686	-0.16121	1.75131
C	-0.70914	-1.28424	2.379911
C	-0.75802	-1.41435	3.769395
C	-1.37036	-0.42855	4.54865
C	-1.93344	0.691292	3.931445
C	-1.8889	0.826096	2.541273
C	1.308421	0.743598	-0.35678
C	1.339358	-0.65656	-0.38432
C	2.546398	-1.34713	-0.40977
C	3.749326	-0.60517	-0.42026
C	3.717341	0.801964	-0.40031
C	2.481997	1.489647	-0.36856
O	0.05406	1.217686	-0.34192
O	0.111183	-1.1866	-0.39279
Cl	2.387196	3.221398	-0.33906
Cl	5.196243	1.710748	-0.40954
Cl	5.267128	-1.44689	-0.44931
Cl	2.523208	-3.08288	-0.41722
H	-1.21952	-3.09584	-0.65366
H	-5.64641	-1.08569	-1.79031
H	-5.29938	-3.53507	-1.99493
H	-3.08971	-4.54231	-1.43954
H	-1.34459	3.130327	-0.08571
H	-3.25991	4.625726	-0.64924
H	-5.42427	3.649525	-1.40343
H	-5.68024	1.19097	-1.62617
H	-0.22101	-2.05421	1.781651
H	-0.31183	-2.2916	4.244429
H	-1.40692	-0.53252	5.636075
H	-2.41176	1.468156	4.533093
H	-2.33536	1.7052	2.075846
P	-1.20273	-0.00643	-0.08088

12 (S_0): *E* = -3152.616760 hartree

Atom	X	Y	Z
Sb	1.124843	-0.09881	0.132597
Cl	-3.051	-2.81681	-0.8617
Cl	-5.68083	-1.0218	-0.76893
Cl	-2.55331	3.337056	0.330161
Cl	-5.42766	2.072509	-0.16951
O	-0.56887	-1.24354	-0.3825
O	-0.355	1.333828	0.135285
C	-1.59248	0.84508	-0.06626
C	-1.70206	-0.53976	-0.34546
C	2.649177	1.418914	0.040218
C	1.319889	-1.03161	2.04885
C	-4.1211	-0.30336	-0.50282
C	2.252184	-0.95393	-1.46336
C	3.411671	-0.1901	-1.71162
C	-2.96481	-1.10732	-0.55232
C	-4.0087	1.071344	-0.23382
C	3.620645	1.064429	-0.92101
C	-2.7384	1.643945	-0.01346
C	4.286907	-0.6437	-2.71213
H	5.199657	-0.09076	-2.94178
C	1.945499	-2.10502	-2.18766
H	1.020682	-2.6488	-1.98227
C	4.715778	1.924865	-1.10502
H	5.491069	1.686435	-1.83564
C	2.745891	2.603024	0.771769
H	1.966666	2.875992	1.487876
C	2.830036	-2.53505	-3.18342
H	2.607129	-3.4336	-3.76384
C	2.298704	-0.58167	2.946418
H	2.962411	0.245313	2.682018
C	3.841069	3.451751	0.570525
H	3.923711	4.383722	1.135163
C	4.82277	3.104193	-0.36281
H	5.679593	3.76351	-0.52291

C	0.467668	-2.09126	2.392524
H	-0.29074	-2.43438	1.685728
C	1.577507	-2.25563	4.542924
H	1.677126	-2.73458	5.520319
C	2.424632	-1.19891	4.194953
H	3.185981	-0.85038	4.897358
C	0.602462	-2.69994	3.644051
H	-0.05991	-3.52543	3.916624
C	3.996562	-1.8049	-3.43475
H	4.689087	-2.13864	-4.21166

1' (S_0): *E* = -2930.086636 hartree

Atom	X	Y	Z
As	-0.00021	-0.00028	-1.20347
C	1.157531	-1.31083	-0.27798
C	1.248407	-2.59237	-0.8472
C	1.911303	-1.02618	0.870964
C	2.059858	-3.57417	-0.27133
H	0.680867	-2.82858	-1.75278
C	2.730161	-2.00654	1.443037
H	1.86303	-0.0338	1.325099
C	2.804568	-3.28201	0.875846
H	2.11644	-4.56763	-0.72442
H	3.312734	-1.77035	2.337761
H	3.445249	-4.04604	1.323943
C	0.556538	1.657879	-0.27879
C	-0.07093	2.17281	0.865928
C	1.62555	2.373171	-0.84471
C	0.369215	3.372339	1.437207
H	-0.90988	1.638263	1.317391
C	2.07064	3.566924	-0.26955
H	2.117164	1.996363	-1.7471
C	1.441214	4.07022	0.873482
H	-0.12984	3.762256	2.328624
H	2.906349	4.109295	-0.71997

H	1.783005	5.007187	1.321002
C	-1.71428	-0.34714	-0.27824
C	-2.86932	0.215364	-0.84754
C	-1.84509	-1.14261	0.870412
C	-4.12549	0.003648	-0.272
H	-2.7898	0.825208	-1.75293
C	-3.10372	-1.36148	1.442126
H	-0.96175	-1.59739	1.324586
C	-4.24525	-0.78773	0.874878
H	-5.01394	0.451722	-0.72513
H	-3.1908	-1.98443	2.336591
H	-5.2274	-0.9605	1.322696

2' (S_0): *E* = -4950.803082 hartree

Atom	X	Y	Z
As	-0.00276	0.000319	-1.74795
F	-1.89431	6.173019	-1.20249
F	6.335824	-0.46943	-0.56261
F	5.710544	-1.59385	-2.30069
F	-3.46966	4.724956	-0.88641
F	-2.36844	4.725721	-2.74803
F	-4.95815	-1.41797	2.354058
F	1.420871	2.717632	2.895029
F	5.32107	0.531756	-2.19856
F	3.799617	-2.76964	2.874155
F	2.362598	4.276308	1.728477
F	1.64849	-2.49434	2.946553
F	-3.0102	-1.32222	3.290708
F	2.494344	-4.12757	1.809377
F	-3.80409	0.418203	2.281786
F	-3.66484	-5.21234	-0.56544
C	1.597289	-0.69797	-0.81349
C	-1.40775	-1.0295	-0.80609
C	2.841419	-0.4099	-1.39544
H	2.899937	0.190683	-2.30662

F	0.554613	4.70631	2.836015
C	-0.1937	1.739081	-0.82026
C	4.023141	-0.87876	-0.81422
C	-2.06267	-0.59394	0.352454
H	-1.80169	0.360367	0.813053
C	1.555874	-1.47957	0.347429
H	0.603143	-1.71816	0.823227
C	-1.24858	3.931101	-0.82461
C	-1.06935	2.66931	-1.40008
H	-1.61625	2.41963	-2.31286
C	-0.53627	4.28977	0.323294
H	-0.66718	5.277583	0.766372
F	-2.22954	-4.88088	-2.15878
C	2.741259	-1.95539	0.922601
C	0.516806	2.101989	0.330774
H	1.205341	1.399477	0.803294
C	-1.7867	-2.25122	-1.3828
H	-1.29841	-2.60811	-2.29314
C	5.355828	-0.59651	-1.47118
C	3.977663	-1.65252	0.349516
H	4.899529	-2.00883	0.810645
C	-3.06883	-1.37635	0.93285
C	0.348729	3.372897	0.89444
F	-4.23958	-4.09959	-2.32862
C	-2.2479	4.89678	-1.42127
C	2.672797	-2.8385	2.148739
C	-3.4376	-2.59509	0.359791
H	-4.22366	-3.20045	0.812578
C	-2.79286	-3.02928	-0.80209
C	1.172646	3.770724	2.098769
C	-3.71873	-0.92093	2.220436
C	-3.23121	-4.31577	-1.46537

3' (S_0): *E* = -3273.401243 hartree

Atom	X	Y	Z

As	0.095768	0.019424	1.547202
O	5.508051	-0.31096	-1.37204
O	-2.61265	4.768653	-1.28763
O	-2.84987	-4.91333	-0.65994
C	-0.86998	-1.50069	0.736307
C	-0.70677	-2.76663	1.332368
H	-0.04622	-2.88096	2.197655
C	1.803675	-0.10068	0.562828
C	-0.75286	1.521514	0.586047
C	-2.50241	3.232351	0.609597
H	-3.34948	3.687786	1.123395
C	2.897779	0.607467	1.077269
H	2.780297	1.20638	1.985979
C	-1.371	-3.88667	0.844388
H	-1.24321	-4.86976	1.302655
C	-1.84444	2.147838	1.201994
H	-2.2006	1.789808	2.173189
C	2.004965	-0.87473	-0.5947
H	1.177508	-1.45054	-1.01623
C	4.153695	0.572858	0.459986
H	4.976825	1.141942	0.893021
C	-0.31477	2.028249	-0.6513
H	0.541648	1.573548	-1.15493
C	-1.73995	-1.39756	-0.35492
H	-1.89983	-0.42971	-0.83611
C	4.335662	-0.19982	-0.69737
C	-2.42341	-2.51482	-0.85418
H	-3.09299	-2.39012	-1.70578
C	-2.05572	3.721552	-0.62755
C	-0.95354	3.110126	-1.25111
H	-0.61584	3.507767	-2.21077
C	3.249289	-0.92566	-1.21714
H	3.410676	-1.52635	-2.11502
C	-2.23926	-3.7702	-0.25633
C	6.641053	0.38633	-0.90756
H	6.479563	1.479704	-0.9031

H	7.459849	0.151613	-1.60115
H	6.933107	0.068094	0.109767
C	-3.71732	5.434197	-0.7199
H	-3.99499	6.234181	-1.41957
H	-3.46916	5.88567	0.257891
H	-4.58267	4.759361	-0.588
C	-3.7367	-4.8729	-1.75415
H	-4.5981	-4.20735	-1.56285
H	-4.10518	-5.89778	-1.89724
H	-3.23377	-4.54189	-2.681

4' (S_0): *E* = -2928.900213 hartree

Atom	X	Y	Z
C	-0.77311	1.333291	-0.46486
C	-1.84799	0.739262	0.237262
C	-1.84799	-0.73926	0.237262
C	-0.77311	-1.33329	-0.46486
As	0.369088	-5E-07	-1.34712
C	-0.65395	2.722565	-0.53885
C	-1.59739	3.535576	0.099403
C	-2.66557	2.954985	0.794339
C	-2.7953	1.566056	0.862284
C	-2.79531	-1.56605	0.862284
C	-2.66557	-2.95498	0.794338
C	-1.59739	-3.53557	0.099402
C	-0.65396	-2.72256	-0.53885
C	1.931061	-1.4E-06	-0.12739
C	1.819589	-3.6E-06	1.272092
C	2.965706	-4E-06	2.070431
C	4.235702	-2.1E-06	1.480527
C	4.355077	1E-07	0.089151
C	3.206031	4E-07	-0.71134
H	0.173215	3.179279	-1.08965
H	-1.50282	4.623478	0.051017
H	-3.40524	3.591911	1.286271

H	-3.63626	1.128922	1.406171
H	-3.63626	-1.12892	1.40617
H	-3.40524	-3.59191	1.28627
H	-1.50283	-4.62348	0.051016
H	0.173209	-3.17928	-1.08965
H	0.833158	-5.1E-06	1.742815
H	2.868497	-5.7E-06	3.159513
H	5.130915	-2.4E-06	2.10796
H	5.343692	1.5E-06	-0.37779
H	3.306932	1.9E-06	-1.80081

5' (S_0): *E* = -3602.473938 hartree

Atom	X	Y	Z
As	-1.07323	-1.74834	0.36371
F	1.879887	3.607814	0.698745
F	0.541898	3.352751	-0.98265
F	2.689639	3.337752	-1.28719
F	4.586595	-1.95125	-0.96219
F	5.346642	-0.47713	0.42839
F	4.313147	-2.23771	1.162458
C	-2.15196	-0.5153	1.446481
C	-3.14426	0.140755	0.680926
C	-2.11045	-1.07571	-1.16273
C	-3.12112	-0.16961	-0.76468
C	0.5428	0.731154	-0.10599
H	-0.41019	1.254384	-0.20385
C	-2.06357	-0.31194	2.824933
H	-1.30242	-0.82952	3.41551
C	0.5706	-0.64822	0.150054
C	1.734059	1.446633	-0.24164
C	3.001441	-0.57461	0.118609
C	-1.97844	-1.45551	-2.49966
H	-1.20305	-2.16494	-2.80212
C	1.805253	-1.29376	0.264531
H	1.847635	-2.36592	0.472952

C	-2.84499	-0.92101	-3.45991
H	-2.74104	-1.20833	-4.50924
C	-2.95565	0.563775	3.454219
H	-2.88568	0.733267	4.531623
C	-3.94094	1.217153	2.704018
H	-4.64016	1.895965	3.198764
C	2.970004	0.795718	-0.13314
H	3.89923	1.355336	-0.24551
C	-4.0404	1.007177	1.326732
H	-4.81744	1.522598	0.757269
C	-3.84829	-0.02357	-3.07463
H	-4.52749	0.387854	-3.82556
C	-3.99116	0.349691	-1.73628
H	-4.78168	1.048532	-1.45265
C	1.707311	2.941736	-0.45842
C	4.319511	-1.30861	0.190303

6' (S_0): *E* = -3424.661857 hartree

Atom	X	Y	Z
As	0.60518	0.204019	-1.41883
F	-1.81905	1.963824	-1.2872
F	-4.92872	-0.58245	1.153428
F	-4.28007	1.692598	-0.20984
F	-3.08755	-2.56967	1.432735
F	-0.64504	-2.32172	0.379682
C	1.356811	1.514159	-0.15516
C	2.749093	3.128595	1.643115
H	3.292253	3.762426	2.348636
C	2.704966	-0.46138	0.330832
C	3.737005	-1.21657	0.910458
H	4.412239	-0.76037	1.638043
C	2.040475	-2.41117	-0.98111
H	1.387259	-2.88118	-1.72075
C	-1.12492	-0.14851	-0.47281
C	0.998078	2.855943	-0.01272

H	0.176488	3.274959	-0.59708
C	-2.10382	0.840636	-0.609
C	2.423534	0.965468	0.593204
C	1.849451	-1.07916	-0.60948
C	1.693234	3.662849	0.895684
H	1.412059	4.711974	1.016995
C	3.117093	1.789632	1.492958
H	3.945407	1.388574	2.081684
C	3.909403	-2.55551	0.554801
H	4.713623	-3.13707	1.012555
C	3.06628	-3.15456	-0.38936
H	3.211277	-4.20156	-0.6669
C	-3.71676	-0.44347	0.630071
C	-1.49362	-1.30557	0.218527
C	-3.38288	0.721594	-0.06577
C	-2.76971	-1.45859	0.773936

7' (S_0): *E* = -3043.338798 hartree

Atom	X	Y	Z
As	-0.43985	-1.1E-06	1.480693
O	5.003934	-1.2E-05	-1.38017
C	-1.43655	1.333031	0.435352
C	-2.39509	-0.73931	-0.41894
C	-1.43656	-1.33303	0.435351
C	1.288652	-4.3E-06	0.528268
C	2.457555	-4.5E-06	1.296482
H	2.391792	-3.4E-06	2.388745
C	-2.39509	0.739314	-0.41894
C	3.83272	-8.2E-06	-0.69738
C	-3.23818	-1.56595	-1.17897
H	-3.9888	-1.12868	-1.84192
C	-1.32865	-2.72238	0.52419
H	-0.59197	-3.179	1.191332
C	3.726393	-6.6E-06	0.700442
H	4.613755	-7.8E-06	1.333932

C	-1.32864	2.722384	0.524191
H	-0.59195	3.178995	1.191334
C	-3.23817	1.565963	-1.17897
H	-3.9888	1.128693	-1.84192
C	2.661315	-8.1E-06	-1.48015
H	2.766602	-9.3E-06	-2.56724
C	1.411318	-6.3E-06	-0.87436
H	0.516469	-6E-06	-1.50201
C	6.22013	1.38E-05	-0.66743
H	6.324972	-0.89794	-0.03187
H	6.324936	0.897977	-0.03187
H	7.022684	2.71E-05	-1.41725
C	-3.119	-2.95487	-1.09397
H	-3.77645	-3.59173	-1.69146
C	-2.16554	-3.53544	-0.24841
H	-2.07792	-4.62337	-0.18807
C	-3.11899	2.954879	-1.09397
H	-3.77644	3.591744	-1.69146
C	-2.16552	3.535446	-0.24841
H	-2.0779	4.623374	-0.18807

8' (S_0): *E* = -3570.296517 hartree

Atom	X	Y	Z
As	0.540122	-9E-07	-1.3825
S	-2.79494	-1.8907	0.782543
S	-2.79491	1.890712	0.782582
C	-0.62399	-1.33263	-0.52242
C	-1.69356	-0.72339	0.121373
C	-1.69355	0.723401	0.121379
C	-0.62398	1.332634	-0.52241
C	-0.70081	-2.75416	-0.4849
C	-1.81228	-3.19921	0.191476
C	-1.81228	3.199219	0.191449
C	-0.70079	2.754162	-0.48489
C	2.0768	-5.4E-06	-0.13335

C	1.934393	-2.3E-05	1.262872
C	3.06354	-2.3E-05	2.084655
C	4.345628	-7.2E-06	1.52118
C	4.494546	9.7E-06	0.132844
C	3.362653	1.03E-05	-0.69188
H	0.031814	-3.42868	-0.9311
H	-2.11783	-4.22744	0.380904
H	-2.11784	4.227452	0.380848
H	0.031825	3.428682	-0.9311
H	0.937118	-3.5E-05	1.710004
H	2.943791	-3.7E-05	3.171436
H	5.227447	-8E-06	2.167241
H	5.492735	2.22E-05	-0.31312
H	3.486556	2.27E-05	-1.77894

9' (S_0): *E* = -1035.715323 hartree

Atom	X	Y	Z
P	-2.2E-05	-1.2E-05	-1.21002
C	0.59239	-1.56206	-0.40261
C	0.19986	-2.77397	-1.00097
C	1.427496	-1.61055	0.726159
C	0.61052	-4.00007	-0.47301
H	-0.43273	-2.75457	-1.89352
C	1.84916	-2.8385	1.247497
H	1.753598	-0.68353	1.202614
C	1.439728	-4.03535	0.653102
H	0.291307	-4.93107	-0.94904
H	2.500773	-2.85802	2.125309
H	1.770503	-4.99359	1.062113
C	1.05658	1.294016	-0.40266
C	0.681137	2.041228	0.72631
C	2.302201	1.560375	-1.00126
C	1.533654	3.020502	1.247578
H	-0.28454	1.859777	1.203034
C	3.15861	2.529195	-0.47339

H	2.601625	1.003008	-1.89395
C	2.774654	3.264729	0.652907
H	1.22483	3.594375	2.125549
H	4.124327	2.718516	-0.94963
H	3.439054	4.030414	1.061845
C	-1.64895	0.267961	-0.40254
C	-2.50328	1.211993	-1.00231
C	-2.10734	-0.42919	0.727827
C	-3.77041	1.469391	-0.47423
H	-2.17103	1.748659	-1.89606
C	-3.38155	-0.18042	1.249321
H	-1.46668	-1.17364	1.205387
C	-4.21441	0.770744	0.653465
H	-4.41792	2.209863	-0.95139
H	-3.72339	-0.73354	2.128373
H	-5.20963	0.963364	1.06257

10’ (S_0): E = -934.760930 hartree

Atom	X	Y	Z
Sb	0.000507	-0.00021	-1.25881
C	-1.23422	-1.4327	-0.15765
C	-0.62347	1.784944	-0.15747
C	1.858171	-0.35257	-0.15702
C	-0.25122	3.038386	-0.67201
H	0.341398	3.104794	-1.59036
C	-0.80844	-2.07954	1.013363
H	0.179792	-1.8677	1.429552
C	4.30251	-0.87175	1.144266
H	5.250972	-1.07204	1.649659
C	2.203155	0.337696	1.015769
H	1.523846	1.085562	1.432837
C	-1.39673	1.738829	1.013378
H	-1.70686	0.776736	1.429192
C	-2.50599	-1.73608	-0.6724
H	-2.85928	-1.25571	-1.59077

C	-0.62971	4.219283	-0.02454
H	-0.32872	5.186484	-0.43648
C	3.417737	0.078952	1.66197
H	3.673056	0.624719	2.574621
C	-1.39634	4.161579	1.143291
H	-1.69722	5.083173	1.648519
C	2.759014	-1.29941	-0.67314
H	2.521471	-1.84398	-1.59291
C	-1.78003	2.920163	1.659349
H	-2.38258	2.868591	2.570537
C	3.970793	-1.56219	-0.0254
H	4.659078	-2.30468	-0.43862
C	-3.34029	-2.65365	-0.02508
H	-4.32851	-2.87578	-0.4372
C	-1.64069	-3.00153	1.659154
H	-1.29533	-3.49776	2.570461
C	-2.90774	-3.28903	1.14285
H	-3.5561	-4.00985	1.647982

11' (S_0): E = -1034.530037 hartree

Atom	X	Y	Z
C	2.601313	2.972436	0.582944
C	1.483935	3.518605	-0.06364
C	0.533324	2.679746	-0.65364
C	0.692178	1.293164	-0.57588
C	1.815664	0.736982	0.082867
C	2.772912	1.588553	0.654805
H	3.34548	3.634286	1.033401
H	1.358809	4.603311	-0.1131
H	-0.32959	3.109206	-1.17013
H	3.649305	1.174955	1.160119
C	0.692213	-1.29315	-0.57589
C	0.533397	-2.67973	-0.65366
C	1.484033	-3.51857	-0.06367
C	2.601396	-2.97238	0.582915
C	2.772957	-1.58849	0.654789
C	1.815685	-0.73694	0.08286
H	-0.32951	-3.10921	-1.17016
H	1.358937	-4.60328	-0.11314
H	3.345582	-3.63421	1.033364
H	3.649338	-1.17487	1.160106
P	-0.35961	-3.9E-06	-1.35952
C	-1.89875	-2.5E-05	-0.31717
C	-3.13499	2.67E-05	-0.98171
C	-1.88161	-8.7E-05	1.088967
C	-4.33354	0.000019	-0.25824
H	-3.15844	0.000072	-2.07507
C	-3.07639	-9.6E-05	1.810111
H	-0.92699	-0.00013	1.621099
C	-4.30518	-4.3E-05	1.137668
H	-5.28947	0.00006	-0.78864
H	-3.05116	-0.00015	2.903126
H	-5.23949	-5E-05	1.705249

12' (S_0): E = -933.572102 hartree

Atom	X	Y	Z
C	2.798292	2.924206	1.011088
C	1.783816	3.560151	0.288123
C	0.837707	2.791483	-0.39945
C	0.897496	1.396344	-0.3546
C	1.921267	0.743288	0.374258
C	2.868884	1.530368	1.052822
H	3.543041	3.518839	1.546485
H	1.731146	4.651625	0.25721
H	0.050191	3.293985	-0.96873
H	3.671936	1.056891	1.622003
C	0.8975	-1.39634	-0.3546
C	0.837716	-2.79148	-0.39945
C	1.783827	-3.56015	0.288117
C	2.798302	-2.9242	1.011083
C	2.868889	-1.53036	1.052819
C	1.92127	-0.74328	0.374257
H	0.050201	-3.29398	-0.96874
H	1.731161	-4.65162	0.257202
H	3.543053	-3.51883	1.546479
H	3.671939	-1.05688	1.622001
Sb	-0.41208	-1E-07	-1.38018
C	-2.04139	-3.2E-06	0.083756
C	-3.36044	4.8E-06	-0.39501
C	-1.82086	-1.3E-05	1.47021
C	-4.44247	3.8E-06	0.494311
H	-3.55737	0.000012	-1.47198
C	-2.90031	-1.4E-05	2.358332
H	-0.80148	-1.9E-05	1.865258
C	-4.21292	-5.6E-06	1.872119
H	-5.46532	1.02E-05	0.107546
H	-2.71629	-2.1E-05	3.436316
H	-5.05547	-6.6E-06	2.568754

B. Optimized by B3LYP-D3BJ/def2svp

$O{=}PPh_3$ (S_0): E =-1110.994177 hartree

Atom	X	Y	Z
P	-1.1E-05	9.1E-06	0.923942
O	0.00014	0.00019	2.429891
C	1.5244	-0.7138	0.218574
C	2.21913	-1.62534	1.027509
C	2.016813	-0.39602	-1.05542
C	3.384531	-2.2312	0.554149
H	1.839342	-1.83611	2.029797
C	3.18244	-1.00602	-1.52596
H	1.501864	0.340764	-1.6757
C	3.864159	-1.92595	-0.72354
H	3.924725	-2.93991	1.186554
H	3.564965	-0.75528	-2.51829
H	4.777686	-2.39917	-1.09183
C	-0.14397	1.677006	0.218388
C	-0.66649	1.944568	-1.05517
C	0.299437	2.734403	1.026642
C	-0.72099	3.258983	-1.52586
H	-1.04789	1.130293	-1.67507
C	0.241516	4.046528	0.553098
H	0.672849	2.510987	2.028588
C	-0.26392	4.309272	-0.7241
H	-1.13028	3.464896	-2.51783
H	0.586233	4.868666	1.184979
H	-0.31081	5.336979	-1.09251
C	-1.38047	-0.9633	0.218685
C	-2.51822	-1.10681	1.026718
C	-1.35067	-1.55087	-1.05428
C	-3.6257	-1.81305	0.55349
H	-2.51162	-0.67076	2.028249
C	-2.46186	-2.2553	-1.52465
H	-0.45445	-1.47512	-1.67381

C	-3.6003	-2.38338	-0.72315
H	-4.51029	-1.92467	1.1852
H	-2.43536	-2.71376	-2.51612
H	-4.46696	-2.93789	-1.09129

1 (S_0): E = -5149.266216 hartree

Atom	X	Y	Z
As	1.250681	-0.06719	-0.04147
Cl	-5.12257	2.082509	-0.35948
Cl	-2.18851	3.313018	-0.52747
Cl	-2.89834	-2.91085	0.076942
Cl	-5.47528	-1.04256	-0.05178
O	-0.34262	-1.31058	-0.2136
O	-0.0595	1.190206	-0.42118
C	2.584404	1.386122	-0.13599
C	-1.33663	0.755972	-0.35964
C	1.438272	-0.5924	1.826782
C	-1.47684	-0.64161	-0.23814
C	-3.88886	-0.34884	-0.16982
C	-2.75854	-1.1911	-0.12329
C	2.244537	2.745656	-0.16455
H	1.196742	3.041613	-0.18284
C	-3.73496	1.041621	-0.3024
C	-2.44027	1.599427	-0.38883
C	3.938179	1.014374	-0.11346
H	4.21844	-0.0417	-0.09033
C	2.057711	-1.25791	-1.34585
C	2.065623	-2.64228	-1.13123
H	1.622444	-3.06332	-0.2287
C	0.769502	-1.722	2.327448
H	0.113823	-2.29427	1.672918
C	2.237774	0.181758	2.681414
H	2.747082	1.070218	2.309753
C	2.599871	-0.71822	-2.51759
H	2.593743	0.360934	-2.68263

C	3.251787	3.716809	-0.17313
H	2.97884	4.774539	-0.20002
C	0.926035	-2.08166	3.667358
H	0.405904	-2.96244	4.05083
C	1.729918	-1.3156	4.515988
H	1.843712	-1.59819	5.565285
C	4.59692	3.341899	-0.14728
H	5.379421	4.104531	-0.15305
C	4.939992	1.986458	-0.11537
H	5.989949	1.684771	-0.09511
C	2.379074	-0.18127	4.022739
H	2.998488	0.429426	4.683568
C	3.155331	-1.56803	-3.47792
H	3.569618	-1.1485	-4.39752
C	2.643437	-3.48213	-2.0844
H	2.663106	-4.56088	-1.91341
C	3.183926	-2.94747	-3.2587
H	3.626101	-3.60995	-4.00651

1 with O=PPh_3 (S_0): *E* = -6260.314432 hartree

Atom	X	Y	Z
As	-1.65455	-1.17362	-0.07134
Cl	1.996866	-2.10306	-3.17092
Cl	4.765266	-2.44265	-1.63793
Cl	4.800154	-2.41068	1.522917
Cl	2.078456	-2.01096	3.117588
O	-0.32767	-1.88587	-1.26895
O	-0.28769	-1.73062	1.243043
C	-2.46482	-0.28189	-1.63286
C	-1.72335	0.034893	-2.77681
C	-2.34859	0.655782	-3.86134
C	-3.71093	0.967657	-3.81019
C	-4.45346	0.642239	-2.67231
C	-3.83228	0.014256	-1.58847
C	-2.72203	1.291963	1.135343

C	-3.13152	2.114792	2.18871
C	-3.16402	1.619489	3.493794
C	-2.78552	0.296362	3.743289
C	-2.36792	-0.52534	2.694424
C	-2.33965	-0.02912	1.382041
C	-2.73467	-2.78408	0.069386
C	-3.93949	-2.77602	0.785552
C	-4.72658	-3.92953	0.847664
C	-4.31329	-5.09637	0.20059
C	-3.11229	-5.10531	-0.51472
C	-2.32538	-3.95379	-0.58541
C	0.870199	-2.04649	-0.72053
C	0.886279	-1.97851	0.692577
C	2.097002	-2.08291	1.380638
C	3.299922	-2.25811	0.661896
C	3.281803	-2.29459	-0.7409
C	2.058526	-2.17412	-1.43533
H	-0.6626	-0.20577	-2.80978
H	-1.76468	0.897817	-4.75312
H	-4.19563	1.454899	-4.65996
H	-5.52046	0.873253	-2.62592
H	-3.41348	3.149026	1.981128
H	-3.47877	2.264068	4.318117
H	-2.80343	-0.09663	4.762774
H	-2.04025	-1.54432	2.898576
H	-4.26836	-1.87448	1.304555
H	-5.66435	-3.91467	1.408382
H	-4.9271	-5.99887	0.253085
H	-2.78516	-6.0146	-1.02479
H	-1.39627	-3.95435	-1.15546
P	0.605818	2.037968	-0.04685
C	-0.5792	3.378978	-0.37942
C	-0.91506	4.358686	0.563815
C	-1.2532	3.337919	-1.61164
C	-1.913	5.293803	0.272915
H	-0.41444	4.37975	1.532852

C	-2.2566	4.263778	-1.89266
H	-1.01485	2.559692	-2.33729
C	-2.58682	5.244577	-0.95022
H	-2.173	6.055691	1.011585
H	-2.78869	4.210151	-2.84493
H	-3.37484	5.969206	-1.16899
C	1.179951	2.225116	1.660379
C	0.790693	1.258179	2.595703
C	1.997467	3.299061	2.050068
C	1.202238	1.379912	3.925156
H	0.18997	0.406135	2.279571
C	2.399567	3.416052	3.380265
H	2.327779	4.035521	1.313409
C	1.99736	2.45768	4.319071
H	0.906612	0.617027	4.647602
H	3.036683	4.249371	3.685632
H	2.319314	2.548069	5.359401
C	2.031943	2.324969	-1.12942
C	2.825295	1.207952	-1.43123
C	2.361183	3.58325	-1.65269
C	3.945702	1.346478	-2.25009
H	2.553165	0.232684	-1.03128
C	3.48784	3.718913	-2.46855
H	1.732957	4.45059	-1.43638
C	4.277614	2.603468	-2.76667
H	4.547841	0.465821	-2.48238
H	3.74531	4.69765	-2.88035
H	5.153914	2.714312	-3.41001
O	0.010444	0.666666	-0.30736
H	-4.42545	-0.23801	-0.70702
H	-2.68744	1.694401	0.125005

4 (S_0): *E* = -5148.081367 hartree

Atom	X	Y	Z
As	-1.16468	-0.03039	-0.04371

Cl	2.723063	-3.03722	-0.33163
Cl	5.426715	-1.34675	-0.4294
Cl	5.281656	1.808396	-0.50248
Cl	2.440497	3.246648	-0.4741
O	0.286547	-1.26269	-0.41177
O	0.165868	1.257514	-0.43282
C	-2.39162	-1.30009	-0.86416
C	-2.17121	-2.65396	-1.10655
C	-3.21647	-3.42276	-1.63153
C	-4.45416	-2.82995	-1.90391
C	-4.6632	-1.46759	-1.66765
C	-3.62546	-0.68348	-1.14972
C	-3.68994	0.777562	-0.88619
C	-4.79211	1.605955	-1.13215
C	-4.69729	2.978466	-0.88247
C	-3.50975	3.537488	-0.39686
C	-2.40359	2.718083	-0.14194
C	-2.5106	1.348276	-0.37312
C	-1.14065	-0.26639	1.875465
C	-1.91177	0.571711	2.692101
C	-1.8961	0.393452	4.077443
C	-1.11309	-0.61468	4.646318
C	-0.34467	-1.44876	3.828985
C	-0.35522	-1.28049	2.442875
C	1.471226	-0.65425	-0.4349
C	1.409179	0.754033	-0.44936
C	2.574105	1.516665	-0.46681
C	3.826648	0.864324	-0.46978
C	3.89142	-0.53922	-0.4414
C	2.705164	-1.30233	-0.41187
H	-1.19452	-3.09112	-0.89772
H	-3.063	-4.48539	-1.83247
H	-5.26674	-3.43489	-2.31311
H	-5.63335	-1.02141	-1.8947
H	-5.7218	1.190563	-1.52592
H	-5.55812	3.621526	-1.08029

H	-3.44309	4.614059	-0.22413
H	-1.4633	3.137651	0.219791
H	-2.52322	1.360991	2.252765
H	-2.49719	1.047284	4.713512
H	-1.10071	-0.75013	5.730406
H	0.269646	-2.23624	4.271533
H	0.242422	-1.92909	1.802037

4 with O=PPh_3 (S_0): E = -6259.128909 hartree

Atom	X	Y	Z
As	0.961863	1.726508	-0.05827
Cl	-2.8082	1.298962	-3.13352
Cl	-5.47808	0.601959	-1.55139
Cl	-5.44259	0.556566	1.610509
Cl	-2.72552	1.155073	3.15447
O	-0.51175	1.879408	-1.27831
O	-0.45797	1.755004	1.252089
C	2.109678	0.987034	-1.45298
C	1.896767	1.005476	-2.82669
C	2.863406	0.440396	-3.66786
C	4.020781	-0.12799	-3.12492
C	4.218351	-0.15786	-1.74216
C	3.252858	0.389956	-0.88909
C	3.290731	0.356536	0.594074
C	4.298063	-0.22898	1.372942
C	4.177417	-0.25395	2.765402
C	3.059656	0.305714	3.394988
C	2.055223	0.909478	2.629371
C	2.181634	0.930744	1.243648
C	1.409803	3.615438	-0.01651
C	2.473963	4.066051	0.776013
C	2.813157	5.421587	0.785431
C	2.091233	6.331364	0.008656
C	1.029248	5.881997	-0.78139
C	0.687783	4.527706	-0.79813

C	-1.68224	1.622611	-0.7049
C	-1.65491	1.567439	0.709291
C	-2.80728	1.2291	1.417562
C	-4.0059	0.957283	0.722162
C	-4.02573	0.995315	-0.68016
C	-2.85568	1.328325	-1.39585
H	0.977994	1.436174	-3.22698
H	2.711406	0.441478	-4.74999
H	4.771535	-0.56857	-3.78511
H	5.11362	-0.62915	-1.33394
H	5.170423	-0.67957	0.896235
H	4.962329	-0.71993	3.366171
H	2.968341	0.268197	4.482906
H	1.174481	1.348835	3.099223
H	3.03968	3.363238	1.389729
H	3.643438	5.767045	1.406181
H	2.355722	7.391565	0.01955
H	0.461676	6.589732	-1.39053
H	-0.13605	4.172602	-1.41773
P	0.226792	-2.06931	-0.01719
C	1.784432	-2.76503	-0.64276
C	2.87236	-3.00362	0.20922
C	1.922737	-2.97626	-2.02411
C	4.078875	-3.47226	-0.3147
H	2.780292	-2.81631	1.2796
C	3.130785	-3.44038	-2.54301
H	1.083192	-2.77295	-2.69216
C	4.207487	-3.6951	-1.68804
H	4.922564	-3.65978	0.353621
H	3.234499	-3.59852	-3.61858
H	5.152485	-4.06254	-2.09548
C	0.088154	-2.52847	1.732692
C	-0.33574	-1.52523	2.614231
C	0.330449	-3.82705	2.208033
C	-0.51872	-1.82136	3.96671
H	-0.51884	-0.52009	2.236944

C	0.153572	-4.11451	3.561672
H	0.664943	-4.61253	1.526751
C	-0.2722	-3.11162	4.441149
H	-0.86187	-1.03655	4.643811
H	0.345734	-5.1238	3.933157
H	-0.41451	-3.34178	5.499871
C	-1.11059	-2.90256	-0.92076
C	-2.12553	-2.0855	-1.43536
C	-1.17905	-4.29451	-1.0825
C	-3.21474	-2.65476	-2.09866
H	-2.04972	-1.0071	-1.3135
C	-2.26733	-4.85995	-1.74844
H	-0.38258	-4.93687	-0.69942
C	-3.28633	-4.04157	-2.25227
H	-4.00206	-2.00458	-2.48586
H	-2.32248	-5.94355	-1.87683
H	-4.13779	-4.4908	-2.76926
O	0.086343	-0.5705	-0.19763

5 (S_0): *E* = -5821.666099 hartree

Atom	X	Y	Z
As	-0.72191	-1.16124	0.329478
Cl	3.389019	0.206916	2.641951
Cl	2.53233	-1.81547	-3.25317
Cl	5.427414	-0.85924	-2.33345
Cl	5.860409	0.159029	0.624657
F	-4.56138	3.070431	-1.36937
O	0.519367	-1.6501	-1.00409
O	0.880597	-0.8791	1.36948
F	-3.61267	1.996894	-2.99001
F	-3.11594	4.077638	-2.62399
F	1.472298	3.66003	1.513447
F	0.301004	5.239306	0.595038
F	-0.35666	4.336601	2.448444
C	4.107108	-0.84457	-1.21004

C	4.301471	-0.39549	0.108281
C	2.832236	-1.28197	-1.63056
C	-1.63485	-1.73735	1.946648
C	3.223708	-0.38211	1.018258
C	1.974832	-0.84282	0.605086
C	-2.85102	-2.37155	1.624845
C	-2.11405	-2.07532	-0.688
C	1.778539	-1.27636	-0.72012
C	-3.11457	-2.56112	0.174383
C	-2.05944	1.120984	-0.8742
H	-2.64103	0.379736	-1.42242
C	-1.2338	-1.53319	3.264918
H	-0.27357	-1.06153	3.475299
C	-1.06961	0.725713	0.031004
C	-2.29641	2.48095	-1.08996
C	-0.56203	3.043182	0.489688
C	-2.19641	-2.23691	-2.06951
H	-1.38747	-1.88151	-2.7101
C	-0.31835	1.686392	0.71728
H	0.459162	1.378046	1.416158
C	-3.32078	-2.87179	-2.61061
H	-3.40299	-3.00851	-3.6911
C	-2.07918	-1.9565	4.297067
H	-1.78301	-1.80936	5.337971
C	-3.29914	-2.57162	3.995765
H	-3.95527	-2.89911	4.805547
C	-1.54681	3.446339	-0.41421
H	-1.71956	4.506426	-0.60095
C	-3.68816	-2.78192	2.668923
H	-4.64043	-3.27084	2.455013
C	-4.3348	-3.33771	-1.76628
H	-5.21075	-3.83165	-2.19307
C	-4.23647	-3.19016	-0.3791
H	-5.03196	-3.57255	0.263326
C	-3.39954	2.909121	-2.02775
C	0.223283	4.076815	1.262628

5 with O=PPh_3 (S_0): *E* = -6932.716818 hartree

Atom	X	Y	Z
As	0.989747	-0.26278	-0.11118
Cl	-0.91411	3.430376	-2.65542
Cl	-2.5914	5.351393	-0.75415
Cl	-2.56338	4.855858	2.368205
Cl	-0.91252	2.405415	3.549724
O	0.562371	1.314423	-1.10963
O	0.509622	0.85602	1.382611
C	0.820854	-1.3985	-1.68711
C	0.738411	-1.0018	-3.01695
C	0.656477	-1.98565	-4.01034
C	0.660954	-3.33986	-3.65904
C	0.724885	-3.72873	-2.31856
C	0.792104	-2.7558	-1.31414
C	0.788719	-3.01845	0.146871
C	0.718274	-4.28146	0.75006
C	0.658033	-4.38702	2.142516
C	0.671714	-3.24174	2.94709
C	0.759386	-1.97477	2.358364
C	0.818324	-1.87729	0.971269
C	2.91075	0.084197	-0.03888
C	3.757007	-0.783	0.658591
C	5.134218	-0.54366	0.689396
C	5.677395	0.555783	0.022977
C	4.828871	1.417645	-0.67532
C	3.450693	1.188812	-0.70662
C	-0.12748	2.197395	-0.39122
C	-0.14429	1.949494	1.00124
C	-0.90236	2.759018	1.846432
C	-1.63865	3.837756	1.310307
C	-1.63541	4.069247	-0.0742
C	-0.87641	3.24184	-0.92898
H	0.719515	0.060108	-3.2664

H	0.58838	-1.69411	-5.06117
H	0.598103	-4.10339	-4.43786
H	0.700789	-4.78861	-2.06107
H	0.697816	-5.18398	0.136719
H	0.59714	-5.37472	2.605768
H	0.613016	-3.33546	4.033742
H	0.772704	-1.06955	2.9666
H	3.353726	-1.65113	1.180299
H	2.793119	1.868452	-1.24824
P	-2.69032	-1.12741	-0.14694
C	-2.6623	-2.72963	-0.99874
C	-2.43337	-3.9237	-0.30008
C	-2.78167	-2.7521	-2.39804
C	-2.3503	-5.1322	-0.99459
H	-2.31213	-3.90939	0.783663
C	-2.69417	-3.96091	-3.08677
H	-2.93931	-1.82089	-2.94607
C	-2.48551	-5.15235	-2.385
H	-2.17484	-6.06048	-0.44604
H	-2.78245	-3.97301	-4.17509
H	-2.42089	-6.09951	-2.92597
C	-3.1611	-1.42575	1.578087
C	-2.42341	-0.75429	2.562105
C	-4.24878	-2.23536	1.942178
C	-2.77305	-0.89352	3.906962
H	-1.5822	-0.1269	2.271002
C	-4.58771	-2.3766	3.287979
H	-4.82776	-2.76076	1.17938
C	-3.85012	-1.70498	4.270569
H	-2.2011	-0.3564	4.666225
H	-5.43131	-3.00952	3.572956
H	-4.12197	-1.8138	5.323296
C	-4.00127	-0.14159	-0.92309
C	-3.70467	1.201255	-1.19179
C	-5.27419	-0.65348	-1.21642
C	-4.67815	2.036356	-1.74366

H	-2.70923	1.57975	-0.96958
C	-6.24415	0.183982	-1.76938
H	-5.50656	-1.70401	-1.02599
C	-5.94781	1.527823	-2.0298
H	-4.4326	3.081597	-1.94317
H	-7.23555	-0.2122	-2.00122
H	-6.71225	2.178528	-2.46127
O	-1.38738	-0.3493	-0.22348
H	6.751393	0.74003	0.047595
C	5.408843	2.57414	-1.45181
C	6.028031	-1.44973	1.498571
F	6.560778	3.008247	-0.91186
F	5.677582	2.222327	-2.72344
F	4.562416	3.614338	-1.50074
F	6.113149	-1.04092	2.77814
F	5.566315	-2.71194	1.519523
F	7.27965	-1.48133	1.010656

6 (S_0): *E* = -5643.837224 hartree

Atom	X	Y	Z
As	1.035065	-0.63362	-0.0673
Cl	-5.49451	-0.46002	-1.63553
Cl	-2.72553	-0.41178	-3.21006
Cl	-2.72226	-1.12171	3.043627
Cl	-5.49298	-0.81617	1.501303
F	1.035117	1.659733	-2.21052
O	-0.36695	-0.76269	-1.34902
F	0.910414	5.420368	0.576457
F	0.964592	4.321468	-1.91161
F	0.937835	3.822574	2.778283
F	1.008181	1.157311	2.51127
O	-0.36575	-1.04739	1.1494
C	-3.99947	-0.63792	-0.77552
C	2.31167	-1.08057	-1.47354
C	4.411	-1.76744	-3.148

H	5.238875	-2.03339	-3.80944
C	-1.5837	-0.76065	-0.79199
C	-2.7818	-0.61595	-1.48877
C	3.51124	-1.71254	0.565973
C	4.572704	-2.21057	1.331233
H	5.516646	-2.48461	0.856571
C	-3.99887	-0.79665	0.62174
C	2.143716	-1.53921	2.587647
H	1.192797	-1.28845	3.055819
C	1.046162	1.304177	0.139445
C	2.138678	-0.97528	-2.85231
H	1.187326	-0.6324	-3.25689
C	1.019828	2.150336	-0.97574
C	3.509743	-1.55999	-0.9113
C	2.314017	-1.35897	1.216327
C	3.201661	-1.32225	-3.69296
H	3.084074	-1.24817	-4.77627
C	4.569318	-1.89111	-1.76457
H	5.513996	-2.25671	-1.35796
C	-1.58341	-0.91997	0.607424
C	4.417172	-2.3728	2.710982
H	5.246502	-2.76771	3.302479
C	3.20855	-2.04998	3.337563
H	3.092864	-2.19978	4.413242
C	0.950941	4.105136	0.436839
C	1.006545	1.896873	1.407205
C	0.981274	3.539227	-0.83971
C	-2.78039	-0.93518	1.320421
C	0.967707	3.283371	1.566043

6 with $O{=}PPh_3$ (S_0): E = -6754.890221 hartree

Atom	X	Y	Z
As	1.430095	-0.11024	-0.07969
Cl	-0.75023	2.914744	-3.21535
Cl	-2.63176	4.95622	-1.66733

Cl	-2.64715	4.965841	1.493518
Cl	-0.80598	2.907126	3.074459
O	0.883483	1.225678	-1.32627
O	0.813975	1.177504	1.202332
C	1.384771	-1.50214	-1.4437
C	1.319015	-1.33331	-2.8213
C	1.280549	-2.47129	-3.63763
C	1.306299	-3.74634	-3.06361
C	1.352278	-3.90395	-1.67558
C	1.378612	-2.777	-0.84754
C	1.374064	-2.79252	0.636013
C	1.342318	-3.93786	1.440943
C	1.300372	-3.8119	2.832951
C	1.295466	-2.54939	3.43564
C	1.338946	-1.39602	2.643064
C	1.378119	-1.53114	1.259834
C	3.317597	0.451635	-0.03984
C	4.347174	-0.4955	-0.05134
C	5.694757	-0.1332	-0.02416
C	6.040447	1.21812	0.016085
C	5.037446	2.187737	0.028881
C	3.694974	1.798925	0.000639
C	0.093318	2.140369	-0.77346
C	0.060507	2.120901	0.640576
C	-0.78835	2.977946	1.336043
C	-1.6055	3.88364	0.624229
C	-1.584	3.890961	-0.77855
C	-0.73246	3.010844	-1.48095
H	1.277633	-0.32874	-3.24452
H	1.227665	-2.36119	-4.72341
H	1.275128	-4.63107	-3.70373
H	1.348769	-4.90613	-1.245
H	1.341217	-4.93004	0.986292
H	1.269532	-4.7101	3.454443
H	1.251999	-2.46216	4.523599
H	1.324727	-0.40249	3.092807

P	-2.16896	-1.3086	0.0248
C	-2.04661	-3.00991	-0.59797
C	-1.75925	-4.087	0.252531
C	-2.16617	-3.22629	-1.98049
C	-1.61681	-5.37231	-0.27446
H	-1.63935	-3.92162	1.323567
C	-2.01937	-4.51081	-2.50202
H	-2.37121	-2.38606	-2.64713
C	-1.75137	-5.5857	-1.64873
H	-1.39646	-6.20925	0.392289
H	-2.10876	-4.67305	-3.57821
H	-1.64066	-6.5927	-2.05819
C	-2.6002	-1.38844	1.783858
C	-1.91519	-0.52085	2.644693
C	-3.61642	-2.21898	2.283261
C	-2.24464	-0.4862	4.001331
H	-1.13066	0.122638	2.24981
C	-3.93466	-2.1855	3.640969
H	-4.15632	-2.89573	1.617377
C	-3.24884	-1.31851	4.500362
H	-1.71424	0.201988	4.662535
H	-4.72212	-2.83446	4.031126
H	-3.50461	-1.29124	5.562365
C	-3.56077	-0.54291	-0.85322
C	-3.36878	0.758172	-1.33504
C	-4.79831	-1.18148	-1.0252
C	-4.41142	1.427417	-1.97944
H	-2.39976	1.234457	-1.20482
C	-5.8377	-0.5101	-1.67042
H	-4.9493	-2.20301	-0.66823
C	-5.64575	0.793888	-2.14424
H	-4.24725	2.443125	-2.34523
H	-6.80178	-1.00548	-1.80753
H	-6.46413	1.314786	-2.64713
O	-0.92553	-0.46226	-0.19316
F	4.076447	-1.80084	-0.08955

F	6.645535	-1.06286	-0.03662
F	7.31648	1.578598	0.042533
F	5.363959	3.475467	0.067955
F	2.796043	2.77813	0.016031

7 (S_0): E = -5262.528248 hartree

Atom	X	Y	Z
As	1.109264	-0.4126	0.136649
Cl	-2.78783	0.786298	2.914021
Cl	-5.35543	-1.35897	-1.42943
Cl	-5.49429	0.076842	1.38176
Cl	-2.51677	-2.06954	-2.68574
O	-0.24107	-1.26893	-0.86848
O	-0.35876	-0.15215	1.39331
O	1.410562	5.376782	-1.69553
C	2.432392	-1.32544	-0.97796
C	3.498067	-1.32147	1.220334
C	2.284694	-0.74927	1.650553
C	1.182008	1.428129	-0.42342
C	0.422255	2.399527	0.240478
H	-0.21594	2.111568	1.076046
C	-3.96137	-0.34576	0.687131
C	3.577903	-1.64704	-0.22725
C	-1.54192	-0.38931	0.834645
C	-1.4833	-1.01469	-0.42804
C	-2.77432	-0.03748	1.384334
C	-3.89943	-0.98054	-0.56485
C	1.294118	4.114358	-1.23413
C	4.50201	-1.55529	2.16772
H	5.455708	-1.99273	1.866134
C	2.051237	-0.43606	2.987588
H	1.089939	-0.01759	3.286396
C	0.472763	3.735683	-0.15948
H	-0.13236	4.469204	0.371958
C	2.337922	-1.63855	-2.33215

H	1.421523	-1.41371	-2.88087
C	4.660822	-2.25993	-0.87026
H	5.564232	-2.51684	-0.3136
C	-2.64816	-1.31119	-1.13046
C	2.060734	3.138969	-1.89799
H	2.692219	3.454174	-2.73028
C	2.004059	1.810901	-1.49806
H	2.60391	1.068481	-2.02591
C	0.662448	6.407399	-1.08507
H	0.927612	6.526977	-0.0199
H	-0.42337	6.224169	-1.16501
H	0.910515	7.331951	-1.62196
C	4.280036	-1.23444	3.510549
H	5.066133	-1.42453	4.245166
C	3.062376	-0.68281	3.923459
H	2.897697	-0.44811	4.977482
C	4.579528	-2.55643	-2.23421
H	5.424773	-3.03854	-2.73103
C	3.423734	-2.25627	-2.96413
H	3.365728	-2.51104	-4.02483

7 with O=PPh_3 (S_0): E = -6373.574574 hartree

Atom	X	Y	Z
As	-1.67658	-0.03786	-0.11239
Cl	0.754424	-2.99649	-3.14757
Cl	2.729095	-4.89476	-1.53026
Cl	2.690181	-4.84354	1.631248
Cl	0.714035	-2.85839	3.140805
O	-0.9936	-1.36352	-1.32323
O	-0.96339	-1.2541	1.209462
C	-1.6073	1.333508	-1.49975
C	-1.46998	1.148743	-2.87087
C	-1.47857	2.271143	-3.70839
C	-1.62508	3.551891	-3.16476
C	-1.74273	3.729914	-1.78408

C	-1.72053	2.617501	-0.93433
C	-1.75287	2.661827	0.548558
C	-1.79987	3.824263	1.330119
C	-1.75246	3.730374	2.724021
C	-1.66222	2.482976	3.352294
C	-1.63072	1.313674	2.583217
C	-1.67897	1.413872	1.195823
C	-3.50765	-0.65743	-0.12434
C	-4.45573	-0.08901	0.731054
C	-5.78884	-0.51033	0.708588
C	-6.18426	-1.5187	-0.18276
C	-5.23243	-2.09312	-1.04404
C	-3.91103	-1.66731	-1.01555
C	-0.16552	-2.21869	-0.73529
C	-0.15924	-2.16782	0.679764
C	0.726203	-2.96541	1.40357
C	1.604684	-3.83734	0.723607
C	1.608927	-3.87263	-0.67876
C	0.720023	-3.05607	-1.41067
H	-1.33579	0.14301	-3.2713
H	-1.36767	2.145608	-4.78826
H	-1.63011	4.424558	-3.82205
H	-1.82772	4.737421	-1.37415
H	-1.85752	4.80502	0.854589
H	-1.78025	4.641339	3.326998
H	-1.61035	2.421338	4.441736
H	-1.55447	0.331985	3.052441
H	-4.16427	0.694508	1.432399
H	-6.50286	-0.04863	1.389801
H	-5.56097	-2.8773	-1.72853
H	-3.17818	-2.11857	-1.68518
P	1.94391	1.351588	0.020955
C	1.726872	3.042892	-0.60735
C	1.345773	4.093906	0.239028
C	1.85347	3.27141	-1.98709
C	1.117986	5.366707	-0.28835

H	1.219508	3.916903	1.307709
C	1.621937	4.543221	-2.50937
H	2.129654	2.449834	-2.65129
C	1.260609	5.593272	-1.65967
H	0.824281	6.183108	0.375653
H	1.717185	4.714326	-3.58373
H	1.082719	6.590371	-2.06982
C	2.360835	1.473821	1.782863
C	1.695073	0.59795	2.650331
C	3.339196	2.349324	2.2801
C	2.008152	0.598238	4.011482
H	0.938225	-0.07836	2.25527
C	3.64129	2.35066	3.641992
H	3.861489	3.034398	1.608501
C	2.976015	1.47411	4.507971
H	1.494254	-0.09716	4.678231
H	4.399854	3.034228	4.030517
H	3.219254	1.473953	5.573336
C	3.385127	0.661193	-0.8425
C	3.268117	-0.65722	-1.30212
C	4.584262	1.365809	-1.02634
C	4.347669	-1.27701	-1.93495
H	2.327048	-1.18538	-1.16269
C	5.660805	0.743914	-1.66072
H	4.676196	2.40046	-0.68729
C	5.543977	-0.57689	-2.11164
H	4.242014	-2.30684	-2.28261
H	6.595073	1.291133	-1.80715
H	6.391029	-1.05885	-2.60592
O	0.751804	0.440636	-0.19261
O	-7.44598	-1.99872	-0.28298
C	-8.44906	-1.47025	0.554203
H	-9.37742	-2.00035	0.304066
H	-8.21902	-1.63347	1.622336
H	-8.59632	-0.38851	0.384603

8 (S_0): *E* = -5789.466432 hartree

Atom	X	Y	Z
As	-1.05163	-0.04048	0.059851
Cl	5.35865	1.878581	-0.4964
Cl	2.511	3.283197	-0.28128
S	-4.56615	-1.64615	-1.94831
Cl	5.532351	-1.27287	-0.61227
S	-4.79862	1.987577	-0.93798
Cl	2.850478	-2.99484	-0.51582
O	0.25267	1.275021	-0.25789
O	0.395322	-1.24481	-0.39422
C	-3.45357	-0.58589	-1.16102
C	-2.42293	1.347344	-0.15065
C	-3.54632	0.809194	-0.75694
C	1.501095	0.781918	-0.35079
C	-2.24926	-1.22365	-0.90521
C	3.991161	-0.48282	-0.51789
C	2.657183	1.557421	-0.37312
C	3.913939	0.919313	-0.46201
C	1.574149	-0.62418	-0.42183
C	-2.21104	-2.57217	-1.35091
H	-1.34173	-3.22126	-1.25201
C	-1.04466	-0.43307	1.951427
C	-2.56264	2.726978	0.159505
H	-1.7802	3.335498	0.613087
C	-3.39964	-2.94237	-1.93539
H	-3.66593	-3.90272	-2.37412
C	2.813853	-1.25925	-0.48746
C	-1.82769	0.334287	2.824292
H	-2.43846	1.15363	2.442495
C	-3.80065	3.209596	-0.20157
H	-4.18835	4.221364	-0.09266
C	-0.25981	-1.48705	2.441398
H	0.346005	-2.07856	1.754499
C	-0.26245	-1.76666	3.809435

H	0.350383	-2.58542	4.193329
C	-1.04289	-1.00411	4.683394
H	-1.04063	-1.22687	5.753019
C	-1.82489	0.044216	4.190531
H	-2.43485	0.642062	4.871599

8 with O=PPh_3 (S_0): *E* = -6900.519262 hartree

Atom	X	Y	Z
As	0.885909	1.67789	-0.03477
Cl	-5.44417	-0.10932	1.448661
Cl	-2.72157	0.21307	3.030579
S	4.37952	0.548177	-2.4102
Cl	-5.58821	0.689234	-1.60101
S	4.64538	-0.11121	1.295007
Cl	-2.94154	1.648876	-3.0864
O	-0.47858	1.222217	1.249797
O	-0.60126	1.841292	-1.22456
C	3.296957	0.868238	-1.09271
C	2.26882	0.881523	1.093844
C	3.382556	0.577658	0.327688
C	-1.68055	1.103198	0.693822
C	2.107548	1.416828	-1.5388
C	-4.10108	0.857681	-0.71749
C	-2.82181	0.628781	1.342234
C	-4.03923	0.510472	0.63829
C	-1.7455	1.440169	-0.68151
C	2.047638	1.566876	-2.94837
H	1.180015	1.953617	-3.48235
C	1.029111	3.575019	0.369336
C	2.434242	0.579024	2.471331
H	1.66689	0.737515	3.226956
C	3.207674	1.143999	-3.55718
H	3.45532	1.152067	-4.61754
C	-2.94225	1.308483	-1.38245
C	1.913451	4.02056	1.360588

H	2.514026	3.304594	1.923694
C	3.670496	0.035439	2.732259
H	4.063161	-0.31719	3.683704
C	0.261915	4.504052	-0.34788
H	-0.42508	4.154872	-1.1193
C	0.381648	5.867961	-0.07172
H	-0.21945	6.587577	-0.63294
C	1.265036	6.311887	0.916445
H	1.35598	7.37959	1.130636
C	2.030484	5.386621	1.630741
H	2.721778	5.727462	2.405366
O	0.478122	-0.59143	-0.66286
P	0.303608	-2.0113	-0.14351
C	0.930052	-2.32362	1.532605
C	2.145744	-2.99363	1.734606
C	0.212815	-1.83725	2.637281
C	2.62542	-3.19452	3.030617
H	2.7194	-3.35716	0.880862
C	0.691187	-2.05069	3.92949
H	-0.71412	-1.28426	2.494859
C	1.894763	-2.73371	4.128696
H	3.574155	-3.71464	3.181133
H	0.121706	-1.67312	4.781917
H	2.267984	-2.90085	5.142148
C	-1.44864	-2.47018	-0.18094
C	-2.0796	-3.26902	0.783682
C	-2.19305	-1.93984	-1.24809
C	-3.45175	-3.51492	0.690978
H	-1.50892	-3.67902	1.618549
C	-3.5586	-2.20089	-1.34102
H	-1.70362	-1.29575	-1.98088
C	-4.19083	-2.97826	-0.36618
H	-3.94738	-4.11583	1.456652
H	-4.13915	-1.76305	-2.1541
H	-5.26787	-3.14875	-0.42271
C	1.210498	-3.13581	-1.24115

C	2.144224	-2.56804	-2.11845
C	1.014928	-4.52421	-1.21725
C	2.89392	-3.39326	-2.96002
H	2.271379	-1.48525	-2.1326
C	1.763411	-5.34298	-2.06384
H	0.276451	-4.96292	-0.54135
C	2.704931	-4.77776	-2.93254
H	3.626072	-2.94845	-3.63781
H	1.611545	-6.42478	-2.04999
H	3.289824	-5.42213	-3.59345

9 (S_0): *E* = -3254.913735 hartree

Atom	X	Y	Z
P	1.288818	-0.07672	0.01451
Cl	-5.36076	-0.99459	0.033082
Cl	-2.8235	-2.92052	-0.01963
Cl	-1.99096	3.319366	0.259213
Cl	-4.95251	2.133156	0.173652
O	0.102864	1.111648	0.221095
O	-0.21662	-1.30376	0.131597
C	-1.20526	0.735034	0.188053
C	1.606954	-0.71493	-1.68157
C	-1.36015	-0.65818	0.132426
C	1.930654	-1.0467	1.426835
C	-2.27877	1.60919	0.196849
C	-3.76097	-0.32701	0.093037
C	2.612722	1.247031	0.071077
C	-3.58393	1.067188	0.15373
C	-2.64962	-1.19736	0.075316
C	2.139488	-0.37791	2.640649
H	1.954247	0.695962	2.712456
C	2.269212	0.104465	-2.6137
H	2.60242	1.101304	-2.32952
C	4.733773	3.100252	0.087326
H	5.5559	3.819993	0.094739

C	3.949253	0.812354	0.116471
H	4.173499	-0.25673	0.145885
C	2.18534	-2.42142	1.332836
H	2.016717	-2.94995	0.394595
C	1.171058	-1.99127	-2.08949
H	0.601301	-2.6108	-1.40089
C	2.591254	-1.08396	3.75729
H	2.740544	-0.56071	4.704502
C	5.001128	1.727298	0.120058
H	6.032754	1.368816	0.152739
C	2.862859	-2.45108	3.658838
H	3.228783	-3.00033	4.529443
C	2.35505	2.62541	0.037766
H	1.326977	2.982617	0.004813
C	2.666059	-3.11537	2.444301
H	2.879339	-4.18368	2.362939
C	3.411234	3.543941	0.048533
H	3.193096	4.61449	0.026248
C	1.432008	-2.44432	-3.38269
H	1.097955	-3.44123	-3.67911
C	2.501017	-0.34497	-3.91479
H	3.005316	0.310668	-4.62818
C	2.095251	-1.62436	-4.29949
H	2.28665	-1.97878	-5.31519

9 with $O{=}PPh_3$ (S_0): E = -4365.955173 hartree

Atom	X	Y	Z
P	-1.99965	-0.89219	-0.07458
Cl	1.284404	-2.37869	-3.21368
Cl	3.922025	-3.36687	-1.71851
Cl	3.980649	-3.42929	1.440022
Cl	1.423255	-2.47876	3.081485
O	-0.91117	-1.65695	-1.22819
O	-0.83088	-1.59826	1.184478
C	-2.70864	0.058872	-1.52553

C	-1.93203	0.450732	-2.62468
C	-2.50164	1.187792	-3.66665
C	-3.85364	1.539148	-3.62886
C	-4.63735	1.141908	-2.54212
C	-4.06736	0.407746	-1.49972
C	-2.47336	1.742288	0.902057
C	-2.66342	2.712198	1.889049
C	-2.77212	2.337253	3.229178
C	-2.68146	0.985529	3.575909
C	-2.46696	0.018928	2.592385
C	-2.37059	0.386726	1.237063
C	-3.25902	-2.21027	0.122922
C	-4.37065	-2.05918	0.96585
C	-5.32269	-3.07657	1.070935
C	-5.17567	-4.25666	0.339203
C	-4.07363	-4.41102	-0.50609
C	-3.12365	-3.3948	-0.61933
C	0.241824	-2.12205	-0.73938
C	0.274216	-2.10122	0.664226
C	1.421484	-2.50129	1.345934
C	2.548357	-2.92092	0.602335
C	2.515974	-2.91346	-0.80183
C	1.348156	-2.50132	-1.48415
H	-0.87874	0.18137	-2.65186
H	-1.8821	1.485426	-4.5168
H	-4.29761	2.112653	-4.44644
H	-5.69803	1.401862	-2.50403
H	-2.7126	3.764448	1.601184
H	-2.9201	3.094403	4.003088
H	-2.76019	0.680646	4.62232
H	-2.35149	-1.02453	2.880622
H	-4.50157	-1.14592	1.545878
H	-6.18278	-2.94304	1.731471
H	-5.9189	-5.05295	0.424928
H	-3.9524	-5.32837	-1.08713
H	-2.27646	-3.51396	-1.29425

P	1.023513	1.854134	-0.06255
C	0.201632	3.465223	-0.28367
C	0.261003	4.494067	0.66492
C	-0.58805	3.624199	-1.43466
C	-0.45748	5.676003	0.459677
H	0.852594	4.367274	1.572967
C	-1.31057	4.800235	-1.63142
H	-0.66162	2.812061	-2.15942
C	-1.24495	5.828938	-0.68429
H	-0.41032	6.47487	1.203475
H	-1.93467	4.909027	-2.52133
H	-1.81338	6.749503	-0.83733
C	1.667513	1.812076	1.631898
C	0.983936	1.028801	2.570625
C	2.807923	2.537523	2.013374
C	1.429673	0.989654	3.893596
H	0.122737	0.438914	2.25953
C	3.244945	2.496248	3.337668
H	3.359857	3.12314	1.274324
C	2.552332	1.725258	4.279004
H	0.900147	0.36867	4.618533
H	4.133704	3.057471	3.63565
H	2.900528	1.689393	5.314182
C	2.464252	1.85598	-1.16799
C	2.974763	0.601909	-1.53548
C	3.06836	3.026616	-1.64723
C	4.08727	0.516299	-2.37201
H	2.489591	-0.30157	-1.17002
C	4.185532	2.937184	-2.48269
H	2.660585	4.004214	-1.37941
C	4.693996	1.685251	-2.84388
H	4.468451	-0.46761	-2.65267
H	4.65614	3.848421	-2.85955
H	5.564612	1.620867	-3.50114
O	0.101187	0.692624	-0.36549
H	-4.69437	0.11073	-0.6573

H	-2.37769	2.054768	-0.13393

10 (S_0): E = -3153.949790 hartree

Atom	X	Y	Z
Sb	-1.23453	-0.1008	-8.1E-05
Cl	5.666428	-0.9695	-8.7E-05
Cl	3.086288	-2.83897	0.000525
Cl	2.377101	3.40764	-0.00193
Cl	5.307797	2.171414	-0.00134
O	0.248311	1.324893	-0.00131
O	0.54995	-1.27701	-0.00043
C	1.506793	0.853305	-0.00111
C	-1.76645	-1.08049	1.829268
C	1.660536	-0.5539	-0.00061
C	-1.76833	-1.08279	-1.82765
C	2.625101	1.68708	-0.00132
C	4.078793	-0.26754	-0.00049
C	-2.64361	1.538076	-0.00042
C	3.920298	1.128015	-0.00103
C	2.946385	-1.10574	-0.00024
C	-2.75654	-0.52873	-2.65197
H	-3.25251	0.404041	-2.37948
C	-2.75426	-0.52573	2.653601
H	-3.25089	0.406418	2.380192
C	-4.54159	3.598332	-0.00063
H	-5.28043	4.403311	-0.00072
C	-4.01492	1.236734	0.000167
H	-4.35846	0.198097	0.00071
C	-1.11229	-2.2659	-2.19933
H	-0.3126	-2.66355	-1.57409
C	-1.10955	-2.26276	2.202101
H	-0.3102	-2.66094	1.576746
C	-3.10254	-1.17184	-3.84405
H	-3.86968	-0.73776	-4.48962
C	-4.96173	2.264815	6.24E-05

H	-6.0274	2.023166	0.000522
C	-2.46482	-2.36	-4.20986
H	-2.73701	-2.86056	-5.14217
C	-2.22449	2.875617	-0.0011
H	-1.15976	3.109861	-0.00153
C	-1.47054	-2.90262	-3.38991
H	-0.96187	-3.82447	-3.68175
C	-3.1772	3.900029	-0.00121
H	-2.8475	4.941849	-0.00175
C	-1.46653	-2.89796	3.393871
H	-0.95719	-3.81916	3.68661
C	-3.09901	-1.16733	3.84686
H	-3.86586	-0.73271	4.492421
C	-2.46042	-2.35466	4.213843
H	-2.73163	-2.85403	5.147078

10 with O=PPh_3 (S_0): *E* = -4265.009583 hartree

Atom	X	Y	Z
Sb	-1.37099	-1.25967	-0.06854
Cl	2.540502	-1.7344	-3.14085
Cl	5.309525	-1.58979	-1.58985
Cl	5.31498	-1.5622	1.572838
Cl	2.555956	-1.62203	3.141981
O	0.201792	-1.90411	-1.3096
O	0.193772	-1.71628	1.303977
C	-2.33419	-0.44983	-1.81584
C	-1.58379	-0.14607	-2.95903
C	-2.21723	0.399316	-4.07923
C	-3.59462	0.647296	-4.061
C	-4.34429	0.329634	-2.9255
C	-3.71522	-0.22605	-1.80569
C	-3.06026	0.956684	1.334561
C	-3.61858	1.647354	2.415424
C	-3.45833	1.162026	3.7153
C	-2.73884	-0.01723	3.935012

C	-2.17957	-0.70971	2.858099
C	-2.34282	-0.22398	1.552547
C	-2.28557	-3.19459	0.064268
C	-3.44977	-3.37666	0.821955
C	-4.06352	-4.63264	0.87249
C	-3.51422	-5.70808	0.169602
C	-2.35169	-5.5272	-0.58648
C	-1.73711	-4.27353	-0.64232
C	1.382396	-1.85871	-0.70814
C	1.377455	-1.77695	0.714832
C	2.593686	-1.68657	1.402171
C	3.816509	-1.66	0.698653
C	3.815207	-1.6995	-0.70318
C	2.593782	-1.78912	-1.40199
H	-0.51083	-0.34271	-2.96698
H	-1.63132	0.631584	-4.97233
H	-4.08556	1.07702	-4.93787
H	-5.42211	0.509995	-2.91004
H	-4.17101	2.572333	2.23542
H	-3.8904	1.704602	4.559784
H	-2.6044	-0.39593	4.951332
H	-1.59164	-1.61192	3.035076
H	-3.88091	-2.54422	1.38372
H	-4.97074	-4.77088	1.466228
H	-3.99216	-6.68999	0.211718
H	-1.92033	-6.36747	-1.13645
H	-0.8323	-4.12669	-1.23545
P	0.258795	2.123627	-0.02319
C	-1.16791	3.198914	-0.3356
C	-1.71438	4.033725	0.648509
C	-1.80373	3.077458	-1.58309
C	-2.88658	4.746294	0.383017
H	-1.24035	4.109466	1.627822
C	-2.98	3.78071	-1.8379
H	-1.39694	2.41116	-2.34444
C	-3.52213	4.616343	-0.85483

H	-3.31157	5.394928	1.152442
H	-3.47792	3.663448	-2.80236
H	-4.44562	5.165313	-1.05399
C	0.845383	2.426925	1.657307
C	0.759067	1.390869	2.595811
C	1.395905	3.669184	2.016387
C	1.206311	1.609263	3.90156
H	0.369597	0.415216	2.304939
C	1.833017	3.879148	3.323176
H	1.491042	4.46585	1.27424
C	1.733811	2.848754	4.26698
H	1.152169	0.794997	4.625921
H	2.262034	4.843138	3.606043
H	2.083915	3.013397	5.288876
C	1.572664	2.600949	-1.16956
C	2.558422	1.635906	-1.42855
C	1.642282	3.862802	-1.77666
C	3.610951	1.929529	-2.29464
H	2.490488	0.654332	-0.96196
C	2.702898	4.153967	-2.63877
H	0.866559	4.60867	-1.58883
C	3.682978	3.189902	-2.89765
H	4.363714	1.164864	-2.49628
H	2.759662	5.134571	-3.11706
H	4.506021	3.421599	-3.57798
O	-0.07612	0.649223	-0.23928
H	-4.31418	-0.48103	-0.92755
H	-3.17861	1.356757	0.326964

11 (S_0): *E* = -3253.732810 hartree

Atom	X	Y	Z
P	-1.21067	-0.00055	-0.15954
Cl	2.457748	-3.08948	-0.45906
Cl	5.220165	-1.48377	-0.41078
Cl	5.179521	1.672666	-0.3763

Cl	2.386322	3.211074	-0.38551
O	0.072992	-1.17245	-0.54771
O	0.037005	1.230288	-0.4775
C	-2.43548	-1.29256	-0.68611
C	-2.24456	-2.67384	-0.76413
C	-3.32831	-3.49879	-1.08581
C	-4.58984	-2.94465	-1.32705
C	-4.78071	-1.56152	-1.26044
C	-3.70009	-0.7311	-0.94709
C	-3.71803	0.745	-0.87039
C	-4.81522	1.578831	-1.10968
C	-4.65641	2.965623	-1.0346
C	-3.41002	3.522269	-0.728
C	-2.30968	2.693171	-0.48149
C	-2.46994	1.30632	-0.54012
C	-1.16463	-0.11147	1.664192
C	-1.73954	0.886721	2.464775
C	-1.68445	0.787194	3.856526
C	-1.05544	-0.30516	4.4591
C	-0.47889	-1.3004	3.664984
C	-0.53174	-1.20784	2.273596
C	1.306698	-0.65241	-0.50553
C	1.285765	0.747885	-0.46991
C	2.466118	1.480443	-0.43143
C	3.69413	0.779836	-0.42151
C	3.713401	-0.62683	-0.44128
C	2.503439	-1.35572	-0.47521
H	-1.25705	-3.09849	-0.58786
H	-3.18521	-4.57967	-1.1532
H	-5.43145	-3.59512	-1.57678
H	-5.76687	-1.13674	-1.45854
H	-5.78921	1.154406	-1.36123
H	-5.51142	3.618373	-1.22619
H	-3.29204	4.607441	-0.68609
H	-1.33286	3.117086	-0.25035
H	-2.23238	1.742816	2.003898

H	-2.13509	1.569348	4.471795
H	-1.01273	-0.38037	5.548258
H	0.018134	-2.15475	4.130203
H	-0.07492	-1.98322	1.658403

11 with $O{=}PPh_3$ (S_0): E = -4364.776757 hartree

Atom	X	Y	Z
P	0.831962	1.835279	-0.11723
Cl	-2.72277	1.028764	-3.26011
Cl	-5.39073	0.287495	-1.69199
Cl	-5.42989	0.417292	1.466493
Cl	-2.76621	1.217741	3.034431
O	-0.48721	1.824101	-1.32724
O	-0.48526	1.812287	1.092727
C	1.99395	1.171397	-1.40005
C	1.791155	1.096265	-2.7777
C	2.811509	0.59432	-3.59468
C	4.022443	0.174394	-3.03408
C	4.21852	0.231018	-1.65249
C	3.198026	0.717298	-0.82902
C	3.2083	0.766872	0.645996
C	4.242796	0.338713	1.485937
C	4.071179	0.38263	2.871969
C	2.874399	0.857102	3.420198
C	1.842804	1.301092	2.585117
C	2.01001	1.254464	1.201153
C	1.159214	3.641166	-0.11991
C	0.615048	4.453719	0.888561
C	0.871187	5.825558	0.90502
C	1.673349	6.404887	-0.08209
C	2.216428	5.60305	-1.08832
C	1.961826	4.229557	-1.10908
C	-1.68299	1.546519	-0.82378
C	-1.68912	1.554099	0.581966
C	-2.82633	1.203377	1.296649

C	-3.99432	0.839381	0.588001
C	-3.98176	0.804594	-0.81582
C	-2.81512	1.157966	-1.53159
H	0.838903	1.413385	-3.20115
H	2.658258	0.528627	-4.67464
H	4.814297	-0.2175	-3.6768
H	5.154856	-0.12492	-1.22009
H	5.174302	-0.0419	1.062409
H	4.874347	0.04088	3.529462
H	2.741078	0.877432	4.504358
H	0.906662	1.664028	3.007774
H	-0.01436	4.007595	1.658403
H	0.440043	6.445569	1.694837
H	1.872834	7.479174	-0.06763
H	2.841953	6.047048	-1.86652
H	2.390442	3.616442	-1.90185
P	0.410106	-1.9895	0.054582
C	2.042351	-2.55466	-0.50743
C	3.123583	-2.63945	0.381947
C	2.241451	-2.816	-1.87243
C	4.38595	-3.00632	-0.08813
H	2.981557	-2.41116	1.438976
C	3.504689	-3.18021	-2.33735
H	1.406173	-2.73004	-2.57046
C	4.576046	-3.28191	-1.4448
H	5.224621	-3.07261	0.608847
H	3.655219	-3.3789	-3.40063
H	5.564769	-3.57019	-1.81003
C	0.266832	-2.41793	1.812768
C	-0.24447	-1.42694	2.660904
C	0.592488	-3.6834	2.325094
C	-0.43244	-1.70215	4.017025
H	-0.48829	-0.44749	2.252538
C	0.409328	-3.9504	3.682154
H	0.996533	-4.45825	1.669676
C	-0.1046	-2.96002	4.52813

H	-0.84143	-0.92757	4.669082
H	0.665991	-4.93387	4.082801
H	-0.25066	-3.1743	5.589669
C	-0.82389	-2.96389	-0.85709
C	-1.91731	-2.2579	-1.37661
C	-0.74373	-4.35454	-1.02278
C	-2.93403	-2.93693	-2.05105
H	-1.95767	-1.17782	-1.25032
C	-1.76085	-5.03022	-1.69906
H	0.114486	-4.90957	-0.63647
C	-2.85644	-4.32308	-2.20992
H	-3.78145	-2.37221	-2.44577
H	-1.6993	-6.11304	-1.83118
H	-3.65033	-4.85807	-2.7368
O	0.134158	-0.51643	-0.16405

12 (S_0): *E* = -3152.755449 hartree

Atom	X	Y	Z
Sb	-1.12617	-0.07114	0.096323
Cl	3.017187	-2.92485	-0.43418
Cl	5.657042	-1.15147	-0.59177
Cl	5.413974	1.998178	-0.5338
Cl	2.542345	3.339159	-0.3128
O	0.539885	-1.28662	-0.31972
O	0.333574	1.342265	-0.22614
C	-2.34189	-1.21153	-1.21932
C	-2.0576	-2.47074	-1.74141
C	-3.00298	-3.08712	-2.56852
C	-4.2045	-2.43092	-2.85538
C	-4.47253	-1.16083	-2.33597
C	-3.53732	-0.52138	-1.50878
C	-3.71696	0.851297	-0.94228
C	-4.84782	1.648547	-1.17471
C	-4.92362	2.938627	-0.64266
C	-3.87625	3.459091	0.123781

C	-2.74323	2.675331	0.370685
C	-2.67754	1.38487	-0.1505
C	-1.16064	-0.61499	2.149757
C	-2.07918	-0.00234	3.011921
C	-2.09187	-0.35693	4.363607
C	-1.19127	-1.31204	4.844897
C	-0.27634	-1.91807	3.978177
C	-0.25539	-1.57383	2.624207
C	1.676278	-0.58991	-0.37274
C	1.570708	0.822423	-0.32604
C	2.720874	1.613431	-0.37447
C	3.990883	1.007059	-0.46459
C	4.099048	-0.39294	-0.49498
C	2.938271	-1.1887	-0.43819
H	-1.10501	-2.95208	-1.51064
H	-2.80116	-4.0738	-2.99138
H	-4.94353	-2.91112	-3.50106
H	-5.41407	-0.67024	-2.58823
H	-5.6755	1.272262	-1.77828
H	-5.8097	3.547546	-0.83669
H	-3.93883	4.474226	0.522405
H	-1.91174	3.075325	0.95569
H	-2.78014	0.74719	2.636975
H	-2.80533	0.116458	5.042199
H	-1.20179	-1.58485	5.902834
H	0.427112	-2.66325	4.356886
H	0.452533	-2.04276	1.938098

12 with O=PPh_3 (S_0): *E* = -4263.814259 hartree

Atom	X	Y	Z
Sb	1.002397	1.552361	-0.03685
Cl	-2.94371	1.402184	-3.10725
Cl	-5.60974	0.629622	-1.56264
Cl	-5.57561	0.442929	1.594085
Cl	-2.87092	0.977505	3.162412

O	-0.64657	1.862651	-1.28993
O	-0.58727	1.614579	1.345367
C	2.305509	0.805392	-1.55545
C	2.125746	0.859826	-2.93379
C	3.078685	0.269862	-3.77253
C	4.194869	-0.3623	-3.21602
C	4.363627	-0.42206	-1.83087
C	3.413395	0.153875	-0.97382
C	3.483115	0.07339	0.517087
C	4.520766	-0.56621	1.214793
C	4.483998	-0.66509	2.60794
C	3.417709	-0.12379	3.334065
C	2.385943	0.536397	2.657423
C	2.42649	0.631967	1.26899
C	1.478999	3.633227	0.120712
C	2.665266	4.0231	0.755359
C	2.993137	5.378981	0.849735
C	2.135947	6.344673	0.314471
C	0.951536	5.95467	-0.31808
C	0.620857	4.600278	-0.41749
C	-1.79317	1.582123	-0.67581
C	-1.76399	1.459574	0.743693
C	-2.93405	1.107495	1.425744
C	-4.13414	0.870755	0.723683
C	-4.15456	0.971	-0.67463
C	-2.9813	1.328702	-1.36684
H	1.239665	1.346746	-3.34804
H	2.949834	0.301477	-4.85726
H	4.939717	-0.82537	-3.86765
H	5.233939	-0.93833	-1.42384
H	5.360343	-1.0033	0.671943
H	5.297048	-1.17307	3.132487
H	3.390651	-0.21522	4.422392
H	1.546836	0.966311	3.208756
H	3.336274	3.273377	1.182794
H	3.918801	5.681366	1.346004

H	2.391326	7.404492	0.391197
H	0.28076	6.708853	-0.73735
H	-0.29831	4.291522	-0.91879
P	0.128455	-2.08426	-0.02796
C	1.602357	-2.87731	-0.72461
C	2.726292	-3.14656	0.070545
C	1.65082	-3.11758	-2.10729
C	3.879015	-3.67576	-0.51196
H	2.707635	-2.93281	1.139561
C	2.809139	-3.63617	-2.68482
H	0.781382	-2.89526	-2.72969
C	3.920667	-3.92258	-1.88635
H	4.751284	-3.88561	0.111195
H	2.845586	-3.81507	-3.76141
H	4.826009	-4.33306	-2.33992
C	0.026318	-2.53381	1.719944
C	-0.39029	-1.53591	2.612161
C	0.295865	-3.83132	2.186815
C	-0.54323	-1.83983	3.966256
H	-0.5884	-0.52657	2.251796
C	0.145762	-4.12467	3.542572
H	0.636289	-4.60821	1.498674
C	-0.27524	-3.12917	4.431916
H	-0.88012	-1.05979	4.651652
H	0.359028	-5.13202	3.907444
H	-0.39442	-3.36325	5.49257
C	-1.33089	-2.73046	-0.88548
C	-1.99206	-1.85934	-1.76361
C	-1.83678	-4.01891	-0.65601
C	-3.16687	-2.26952	-2.3977
H	-1.59254	-0.86064	-1.93271
C	-3.00367	-4.42724	-1.30234
H	-1.33616	-4.69673	0.038322
C	-3.67199	-3.55093	-2.16605
H	-3.69179	-1.57003	-3.05069
H	-3.40337	-5.42742	-1.12

H	-4.59684	-3.86854	-2.65344
O	0.12915	-0.5711	-0.22213

Cartesian coordinates of optimized geometries formed during the hydrolysis reactions

Hydrolysis of **1**

1

E at B3LYP/6-31G** = -5148.65080876 Hartree

E at B3LYP/SDD + 6-31G**//B3LYP/6-31G** = -2921.00653886 Hartree

Atom	X	Y	Z
As	-1.22695	-0.01462	0.035326
Cl	5.191323	2.017012	0.207499
Cl	2.251433	3.294087	0.339415
Cl	2.867825	-2.96932	-0.01308
Cl	5.495001	-1.13573	0.029486
O	0.349171	-1.30487	0.175131
O	0.115584	1.212087	0.309517
C	-2.52207	1.452916	0.203764
C	1.385229	0.743114	0.235983
C	-1.56437	-0.58598	-1.78322
C	1.498221	-0.65654	0.166002
C	3.912042	-0.40672	0.111219
C	2.768789	-1.23147	0.09504
C	-2.19842	2.807997	0.06301
H	-1.17077	3.10431	-0.10653
C	3.78175	0.989905	0.187901
C	2.495897	1.568623	0.249861
C	-3.85874	1.094721	0.429764
H	-4.13594	0.051829	0.549348
C	-1.98257	-1.20163	1.355417
C	-2.56125	-2.40692	0.954645
H	-2.57653	-2.6901	-0.09291
C	-0.97293	-1.75184	-2.29342
H	-0.29017	-2.32206	-1.6767
C	-2.42348	0.166753	-2.59552

H	-2.88177	1.074351	-2.222
C	-1.95781	-0.83201	2.701687
H	-1.51893	0.115321	3.002401
C	-3.19379	3.783326	0.149758
H	-2.92726	4.830874	0.045092
C	-1.25549	-2.16291	-3.59529
H	-0.79705	-3.06836	-3.98096
C	-2.11262	-1.41134	-4.40076
H	-2.32475	-1.7313	-5.41667
C	-4.52129	3.416728	0.373103
H	-5.29309	4.177855	0.440681
C	-4.85364	2.067999	0.509959
H	-5.88422	1.773753	0.685261
C	-2.69036	-0.24378	-3.9013
H	-3.35128	0.3501	-4.52517
C	-2.50511	-1.68602	3.65809
H	-2.48167	-1.40689	4.707019
C	-3.11654	-3.25221	1.916753
H	-3.57065	-4.19014	1.61149
C	-3.08556	-2.89463	3.265634
H	-3.514979	-3.556273	4.011793

H_2O

E at B3LYP/6-31G** = -76.4197455013 Hartree

E at B3LYP/SDD + 6-31G**//B3LYP/6-31G** = -76.4181668163 Hartree

Atom	X	Y	Z
O	0.000000	0.000000	0.119179
H	0.000000	0.759326	-0.476716
H	0.000000	-0.759326	-0.47671

H_2O-adduct in **1**

E at B3LYP/6-31G** = -5225.10094352 Hartree

E at B3LYP/SDD + 6-31G**//B3LYP/6-31G** = -2997.44463240 Hartree

Atom	X	Y	Z

Cl	5.288439	1.555962	-0.15456
Cl	2.521649	3.172197	-0.19568
Cl	2.42554	-3.10578	-0.72228
Cl	5.240389	-1.60448	-0.41481
O	0.12186	-1.18408	-0.7897
O	0.162624	1.349163	-0.56751
C	-2.50953	1.530388	-0.42404
C	1.360351	0.763507	-0.51351
C	-2.50756	-1.46398	-0.34087
C	1.343556	-0.63961	-0.6448
C	3.75488	-0.69176	-0.45232
C	2.525938	-1.36907	-0.59544
C	-2.17422	2.846505	-0.07334
H	-1.1907	3.071174	0.320023
C	3.775419	0.707757	-0.33351
C	2.568473	1.436166	-0.35819
C	-3.75313	1.272506	-1.01036
H	-4.01413	0.270008	-1.32706
C	-0.83372	-0.08269	1.726931
C	-0.25997	-1.27976	2.174016
H	-0.08039	-2.08684	1.472026
C	-3.40284	-1.65849	0.717223
H	-3.3759	-1.00762	1.585871
C	-2.55291	-2.30484	-1.45258
H	-1.8733	-2.15536	-2.28117
C	-1.07324	0.957939	2.627125
H	-1.52971	1.882919	2.294414
C	-3.09772	3.876522	-0.25416
H	-2.83172	4.889963	0.031017
C	-4.33386	-2.6956	0.66461
H	-5.02329	-2.84361	1.490483
C	-4.37198	-3.54247	-0.4443
H	-5.09423	-4.35244	-0.48495
C	-4.34855	3.607919	-0.81163
H	-5.06396	4.412048	-0.9566
C	-4.67036	2.30637	-1.19762

H	-5.63307	2.093991	-1.65274
C	-3.48311	-3.34433	-1.50206
H	-3.51142	-3.99926	-2.36774
C	-0.73181	0.80478	3.971733
H	-0.9191	1.614763	4.670172
C	0.083971	-1.42618	3.515986
H	0.536324	-2.35202	3.858004
C	-0.14969	-0.38352	4.415357
H	0.119607	-0.49826	5.461126
O	-1.21972	0.249076	-2.76231
H	-0.45317	-0.34335	-2.71599
As	-1.26598	0.039249	-0.15202
H	-0.84537	1.122643	-2.565067

TS1 in **1**

E at B3LYP/6-31G** = -5225.10094352 Hartree

Imaginary frequency: 970.7 *i*cm^{-1}

E at B3LYP/SDD + 6-31G**//B3LYP/6-31G** = -2997.44463240 Hartree

Atom	X	Y	Z
Cl	5.093017	1.789333	-0.02333
Cl	2.2189	3.165431	-0.26102
Cl	2.694135	-3.07911	-0.84067
Cl	5.331482	-1.35761	-0.29523
O	0.249796	-1.40836	-1.07413
O	0.06719	1.238547	-0.86666
C	-2.64346	1.531261	-0.35377
C	1.284594	0.685024	-0.75535
C	-2.65182	-1.46438	-0.21971
C	1.394596	-0.71886	-0.87431
C	3.782843	-0.57406	-0.46034
C	2.632411	-1.34248	-0.71413
C	-3.49816	1.654178	-1.45624
H	-3.4373	0.940442	-2.27027
C	3.676748	0.823319	-0.34198
C	2.422948	1.445079	-0.46828

C	-2.74869	2.437948	0.704546
H	-2.11066	2.346105	1.575202
C	-0.61506	-0.10569	1.476105
C	-0.61817	-1.35671	2.099305
H	-1.08644	-2.20908	1.621515
C	-2.42829	-2.70752	-0.81477
H	-1.52539	-2.89555	-1.38091
C	-3.80241	-1.25719	0.549492
H	-3.98274	-0.29867	1.025707
C	0.052864	0.969106	2.077704
H	0.131794	1.919323	1.560874
C	-4.42806	2.691106	-1.50891
H	-5.08294	2.782557	-2.37019
C	-3.36669	-3.72968	-0.66031
H	-3.18981	-4.69364	-1.12801
C	-4.52178	-3.51879	0.093881
H	-5.2492	-4.31656	0.211291
C	-4.51913	3.605013	-0.45743
H	-5.24454	4.412049	-0.49916
C	-3.68251	3.473651	0.650947
H	-3.75415	4.175453	1.47632
C	-4.73602	-2.28211	0.703601
H	-5.6289	-2.1118	1.297851
C	0.648737	0.809897	3.328048
H	1.159545	1.648805	3.790721
C	-0.01491	-1.51455	3.346795
H	-0.02175	-2.48768	3.828427
C	0.610438	-0.43122	3.966095
H	1.083719	-0.55828	4.935207
O	-1.3637	-0.26675	-2.35184
H	-0.40982	-0.95364	-1.96108
As	-1.40726	0.051123	-0.30419
H	-0.96258	0.564791	-2.65616

OH-adduct in **1**

E at B3LYP/6-31G** = -5225.08919297 Hartree

E at B3LYP/SDD + 6-31G**//B3LYP/6-31G** = -2997.43577303 Hartree

Atom	X	Y	Z
Cl	4.969118	1.96311	0.165494
Cl	2.046019	3.126634	-0.32044
Cl	3.014444	-3.05251	-0.84632
Cl	5.451388	-1.15943	-0.05635
O	0.512695	-1.65897	-1.26905
O	0.081521	1.11388	-1.02794
C	-2.62322	1.612938	-0.23378
C	1.29494	0.593828	-0.85838
C	-2.893	-1.42083	-0.24737
C	1.540322	-0.79693	-0.98428
C	3.873691	-0.48574	-0.36564
C	2.805031	-1.32584	-0.7206
C	-3.29889	2.102019	-1.35728
H	-3.21238	1.5862	-2.30717
C	3.65695	0.899007	-0.26908
C	2.378162	1.422788	-0.5052
C	-2.76796	2.263358	0.99566
H	-2.26133	1.892993	1.879415
C	-0.61364	-0.30813	1.261466
C	-0.60794	-1.5836	1.829553
H	-1.12812	-2.40554	1.353522
C	-2.65943	-2.67505	-0.82183
H	-1.76005	-2.85763	-1.39882
C	-4.04605	-1.21626	0.515449
H	-4.23765	-0.25088	0.974147
C	0.094752	0.736917	1.868546
H	0.130805	1.712538	1.39695
C	-4.08971	3.245202	-1.2564
H	-4.60456	3.621324	-2.13511
C	-3.58288	-3.70669	-0.65176
H	-3.39607	-4.67682	-1.10269
C	-4.74173	-3.49358	0.0974
H	-5.46115	-4.29665	0.227388

C	-4.2217	3.899732	-0.03062
H	-4.83896	4.789721	0.046869
C	-3.56561	3.403552	1.095995
H	-3.66938	3.903482	2.054124
C	-4.97141	-2.2479	0.6823
H	-5.87041	-2.07643	1.26704
C	0.771198	0.513117	3.066201
H	1.31599	1.326926	3.534643
C	0.085734	-1.80549	3.019729
H	0.09731	-2.79955	3.456113
C	0.769658	-0.75955	3.640831
H	1.311318	-0.93817	4.564875
O	-1.57977	-0.26131	-2.24159
H	-0.07735	-1.27492	-1.95233
As	-1.57993	0.018153	-0.41354
H	-1.01622	0.47164	-2.54968

TS2 in **1**

E at B3LYP/6-31G** = -5225.08422702 Hartree

Imaginary frequency: 270.8 *i*cm^{-1}

E at B3LYP/SDD + 6-31G**//B3LYP/6-31G** = -2997.43261389 Hartree

Atom	X	Y	Z
Cl	2.115912	3.054819	-0.17639
Cl	3.093494	-3.10854	-0.83145
Cl	5.561014	-1.21404	-0.10369
O	0.534544	-1.70155	-1.08688
O	0.164344	1.061351	-0.94586
C	-2.46709	1.721509	-0.25521
C	1.352866	0.530484	-0.74294
C	-3.11469	-1.28178	-0.35984
C	1.606778	-0.86022	-0.85068
C	3.965991	-0.54685	-0.32979
C	2.885233	-1.38208	-0.64974
C	-2.77503	2.468516	-1.39572
H	-2.55218	2.066351	-2.37779

C	3.733435	0.833312	-0.18909
C	2.447571	1.353949	-0.38179
C	-2.769	2.233011	1.010576
H	-2.5279	1.669306	1.905623
C	-0.77307	-0.45728	1.210817
C	-0.86562	-1.75071	1.7275
H	-1.39615	-2.52479	1.186194
C	-3.02458	-2.49938	-1.04327
H	-2.18174	-2.68674	-1.69923
C	-4.208	-1.04893	0.479323
H	-4.29359	-0.11146	1.020939
C	-0.06967	0.535673	1.902895
H	0.024996	1.526499	1.472958
C	-3.37502	3.720143	-1.27011
H	-3.60673	4.297082	-2.16021
C	-4.02503	-3.46218	-0.90618
H	-3.94843	-4.40178	-1.44556
C	-5.12134	-3.21681	-0.07759
H	-5.90179	-3.96458	0.028302
C	-3.67566	4.229493	-0.00541
H	-4.14324	5.204885	0.090363
C	-3.37715	3.482706	1.134401
H	-3.60893	3.87317	2.120683
C	-5.21255	-2.00786	0.61402
H	-6.06481	-1.81044	1.257618
C	0.518511	0.236129	3.130348
H	1.060687	1.007661	3.668304
C	-0.25816	-2.04819	2.947676
H	-0.31895	-3.05637	3.346049
C	0.428336	-1.05669	3.650738
H	0.900053	-1.29322	4.599853
O	-1.53845	-0.24865	-2.24374
H	0.584034	-2.06118	-1.98372
As	-1.65071	0.002454	-0.4731
H	-0.74139	0.267795	-2.45858
Cl	2.115912	3.054819	-0.17639

OH-adduct isomer in **1**

E at B3LYP/6-31G** = -5225.09302427 Hartree

E at B3LYP/SDD + 6-31G**//B3LYP/6-31G** = -2997.44978668 Hartree

Atom	X	Y	Z
Cl	4.3136	2.214846	0.98642
Cl	1.418334	2.940601	-0.12033
Cl	3.711835	-2.82106	-1.11917
Cl	5.477733	-0.70234	0.496828
O	1.096344	-1.70889	-2.04363
O	0.133049	0.715231	-1.58226
C	-2.36502	1.60355	-0.2662
C	1.335959	0.453383	-1.15713
C	-3.39892	-1.20541	0.016725
C	1.900088	-0.83576	-1.37304
C	3.917779	-0.24276	-0.13796
C	3.148797	-1.17125	-0.86336
C	-1.88391	2.653627	-1.05528
H	-1.13173	2.456894	-1.8062
C	3.398446	1.041275	0.069025
C	2.129194	1.373799	-0.43433
C	-3.29441	1.859748	0.752196
H	-3.69025	1.053861	1.360579
C	-0.53005	-0.79421	0.795077
C	-0.1112	-2.1278	0.80333
H	-0.53811	-2.83575	0.10036
C	-4.43538	-1.38441	-0.908
H	-4.32129	-1.01736	-1.92265
C	-3.54862	-1.69546	1.318656
H	-2.75088	-1.57391	2.044915
C	0.018254	0.14145	1.673924
H	-0.28645	1.181774	1.628723
C	-2.34712	3.94986	-0.83221
H	-1.97464	4.760871	-1.45027
C	-5.60159	-2.0505	-0.53503

H	-6.397	-2.19159	-1.26059
C	-5.74544	-2.53663	0.766652
H	-6.65518	-3.05469	1.055391
C	-3.26377	4.208335	0.187804
H	-3.61137	5.222238	0.362973
C	-3.73305	3.162828	0.983871
H	-4.44529	3.356071	1.780163
C	-4.71862	-2.35813	1.693695
H	-4.82369	-2.73767	2.705669
C	1.008956	-0.26491	2.567678
H	1.460273	0.461514	3.2357
C	0.879313	-2.52398	1.699154
H	1.226333	-3.55232	1.700862
C	1.442547	-1.59158	2.575125
H	2.230642	-1.89853	3.255514
O	-1.74928	-0.85868	-2.12516
H	1.567473	-2.54859	-2.15088
As	-1.80892	-0.22758	-0.49652
H	-0.8844	-0.48935	-2.43264

Oxide product in **1**

E at B3LYP/6-31G** = -5225.09954107 Hartree

E at B3LYP/SDD + 6-31G**//B3LYP/6-31G** = -2997.46104781 Hartree

Atom	X	Y	Z
Cl	4.009803	2.001256	1.311447
Cl	1.508665	2.935193	-0.4148
Cl	3.746095	-2.87627	-1.18505
Cl	5.115703	-0.95231	0.959556
O	1.47664	-1.58291	-2.64084
O	0.513014	0.901119	-2.25152
C	-2.70132	1.485699	-0.37115
C	1.57083	0.491621	-1.54584
C	-3.21032	-1.52338	0.171951
C	2.099905	-0.80656	-1.72458
C	3.794929	-0.37311	-0.02079

C	3.189281	-1.22477	-0.95821
C	-2.07682	2.544152	-1.04426
H	-1.17117	2.370136	-1.61541
C	3.297706	0.926151	0.137927
C	2.194097	1.345946	-0.62585
C	-3.86189	1.71414	0.376697
H	-4.35076	0.896711	0.89784
C	-0.53468	-0.26382	0.909413
C	0.293373	-1.38953	1.001109
H	0.160516	-2.21293	0.305025
C	-3.92206	-2.26557	-0.77513
H	-3.70331	-2.12928	-1.82986
C	-3.44811	-1.71281	1.537191
H	-2.87672	-1.15685	2.275352
C	-0.35942	0.817255	1.776515
H	-0.98956	1.696015	1.691641
C	-2.62437	3.824808	-0.97064
H	-2.14061	4.644323	-1.49332
C	-4.88304	-3.18466	-0.35462
H	-5.43383	-3.76426	-1.08916
C	-5.13194	-3.36216	1.00825
H	-5.88081	-4.07855	1.332917
C	-3.78468	4.052732	-0.22766
H	-4.20693	5.051933	-0.1738
C	-4.404	2.997887	0.445073
H	-5.30755	3.172411	1.021541
C	-4.41417	-2.62797	1.954867
H	-4.59931	-2.77463	3.014706
C	0.65749	0.774683	2.732167
H	0.813803	1.622204	3.391705
C	1.306224	-1.4264	1.955867
H	1.967445	-2.28521	2.012325
C	1.48838	-0.34248	2.819595
H	2.293959	-0.36263	3.546695
O	-1.38217	-0.7368	-1.94896
H	1.885819	-2.46079	-2.6496

As	-1.9029	-0.26376	-0.43222
H	-0.20217	0.159351	-2.3019

Hydrolysis of **4**

4

E at B3LYP/6-31G** = -5147.45799733 Hartree

E at B3LYP/SDD + 6-31G**//B3LYP/6-31G** = -2919.81551537 Hartree

Atom	X	Y	Z
As	-1.20424	0.011748	-0.12496
Cl	2.478761	-3.16684	-0.5223
Cl	5.280956	-1.61383	-0.49888
Cl	5.29564	1.557641	-0.49862
Cl	2.504712	3.134812	-0.5273
O	0.147457	-1.27219	-0.58648
O	0.158289	1.265045	-0.60089
C	-2.54396	-1.31548	-0.54137
C	-2.40371	-2.69913	-0.58429
C	-3.52227	-3.49643	-0.84055
C	-4.76625	-2.89995	-1.05678
C	-4.90451	-1.51119	-1.03132
C	-3.78892	-0.70734	-0.78042
C	-3.78337	0.776875	-0.75935
C	-4.89469	1.595985	-0.97856
C	-4.74631	2.983647	-0.95979
C	-3.49732	3.563439	-0.72676
C	-2.38407	2.750718	-0.49839
C	-2.53375	1.368339	-0.50588
C	-0.89781	-0.00716	1.765065
C	-0.3928	1.14124	2.38343
C	-0.11544	1.125152	3.749484
C	-0.33529	-0.03629	4.49301
C	-0.82863	-1.1852	3.871186
C	-1.10602	-1.17452	2.504692
C	1.362656	-0.71639	-0.55383

C	1.372122	0.691617	-0.56494
C	2.570858	1.391825	-0.54286
C	3.788752	0.680428	-0.5266
C	3.781553	-0.72407	-0.52401
C	2.557754	-1.4253	-0.53735
H	-1.42948	-3.15038	-0.43624
H	-3.42103	-4.5765	-0.87855
H	-5.63538	-3.51954	-1.25685
H	-5.87674	-1.0645	-1.21228
H	-5.87123	1.162549	-1.1687
H	-5.61139	3.615842	-1.13645
H	-3.38912	4.643555	-0.7278
H	-1.40803	3.192235	-0.33411
H	-0.20172	2.032955	1.795932
H	0.279234	2.015043	4.230061
H	-0.11676	-0.04785	5.556651
H	-0.9916	-2.09068	4.447599
H	-1.48567	-2.068454	2.020923

H_2O-adduct in **4**

E at B3LYP/6-31G** = -5223.90244605 Hartree

E at B3LYP/SDD + 6-31G**//B3LYP/6-31G** = -2996.25370316 Hartree

Atom	X	Y	Z
As	-1.16032	-0.02159	-0.10266
Cl	2.512068	-3.17797	-0.44272
Cl	5.321275	-1.64294	-0.39339
Cl	5.35614	1.52875	-0.40418
Cl	2.574104	3.121183	-0.47867
O	0.195437	-1.28358	-0.54904
O	0.217361	1.274159	-0.57954
C	-2.52627	-1.34196	-0.40404
C	-2.38884	-2.72288	-0.47896
C	-3.52203	-3.51818	-0.66861
C	-4.77856	-2.92166	-0.79446
C	-4.91442	-1.53378	-0.74419

C	-3.78375	-0.73231	-0.55774
C	-3.77835	0.752281	-0.53119
C	-4.90174	1.57505	-0.66972
C	-4.7522	2.962693	-0.66142
C	-3.48981	3.543183	-0.51672
C	-2.36203	2.730784	-0.36885
C	-2.51441	1.348848	-0.3681
C	-0.81479	0.000968	1.792904
C	-0.27782	1.152483	2.378551
C	0.005546	1.171675	3.743278
C	-0.23743	0.039552	4.523505
C	-0.76197	-1.11405	3.937787
C	-1.04578	-1.13621	2.572484
C	1.406787	-0.72386	-0.50509
C	1.427062	0.68526	-0.52275
C	2.630798	1.376562	-0.48097
C	3.844753	0.659792	-0.44696
C	3.82785	-0.74429	-0.4393
C	2.599922	-1.43737	-0.46719
H	-1.40646	-3.17384	-0.39926
H	-3.42294	-4.59758	-0.72726
H	-5.65871	-3.54016	-0.94291
H	-5.89619	-1.08524	-0.8571
H	-5.8903	1.142882	-0.78749
H	-5.62802	3.594744	-0.77381
H	-3.38363	4.623605	-0.52219
H	-1.37668	3.170893	-0.26489
H	-0.07128	2.025183	1.768822
H	0.423789	2.066249	4.194671
H	-0.01364	0.054464	5.586077
H	-0.94477	-1.99816	4.540998
H	-1.45073	-2.03579	2.12048
O	-1.1415	0.184114	-2.73103
H	-1.98154	0.644381	-2.86616
H	-0.51506	0.894468	-2.5166

TS1 in **4**

E at B3LYP/6-31G** = -5223.87713749 Hartree

Imaginary frequency: 825.9 *i*cm^{-1}

E at B3LYP/SDD + 6-31G**//B3LYP/6-31G** = -2996.22319335 Hartree

Atom	X	Y	Z
As	1.297333	0.028693	-0.39709
Cl	-5.39053	-1.37408	-0.14112
Cl	-2.76407	-3.135	-0.6168
Cl	-2.26776	3.132073	-0.44439
Cl	-5.13958	1.782821	-0.07948
O	-0.13427	1.168735	-0.95813
O	-0.3191	-1.49524	-0.99918
C	2.659172	-1.34809	-0.25382
C	-1.46641	-0.78306	-0.82545
C	2.662003	1.337516	-0.40906
C	-1.34308	0.6237	-0.77877
C	-3.73044	0.794409	-0.35363
C	-2.47772	1.40398	-0.53816
C	2.517887	-2.72943	-0.25407
H	1.539472	-3.1808	-0.38557
C	-3.84398	-0.607	-0.38328
C	-2.69876	-1.3933	-0.60396
C	3.922954	-0.73716	-0.12397
C	0.581084	-0.00327	1.419452
C	0.394371	1.203503	2.100614
H	0.659933	2.143981	1.629203
C	2.529106	2.711147	-0.55805
H	1.550415	3.145222	-0.73291
C	3.924636	0.7453	-0.20745
C	0.195888	-1.20835	2.009764
H	0.302252	-2.14003	1.466098
C	3.651117	-3.53208	-0.09405
H	3.556452	-4.61358	-0.09246
C	3.663237	3.52335	-0.48777
H	3.570305	4.598471	-0.6043

C	4.9173	2.94749	-0.27129
H	5.798895	3.579051	-0.21498
C	4.906602	-2.93963	0.061723
H	5.786008	-3.56356	0.189762
C	5.048529	-1.55116	0.043668
H	6.034548	-1.11112	0.154841
C	5.054662	1.56521	-0.1351
H	6.038403	1.135221	0.023445
C	-0.34192	-1.21097	3.296685
H	-0.64441	-2.1486	3.753193
C	-0.13954	1.198132	3.388681
H	-0.27881	2.135349	3.919049
C	-0.50711	-0.00895	3.987191
H	-0.93066	-0.01137	4.987164
O	1.206866	-0.39147	-2.39914
H	1.973343	-0.95049	-2.60243
H	0.279131	-1.12733	-1.92361

OH-adduct in **4**

E at B3LYP/6-31G** = -5223.87971920 Hartree

E at B3LYP/SDD + 6-31G**//B3LYP/6-31G** = -2996.23686687 Hartree

Atom	X	Y	Z
As	1.26154	-0.10698	-0.17779
Cl	-5.9635	-0.15856	-0.80692
Cl	-4.15484	-2.76031	-0.40761
Cl	-1.56923	2.902417	0.392442
Cl	-4.65556	2.71004	-0.4083
O	-0.33187	0.299924	0.903691
O	-1.34071	-2.11418	0.390586
C	2.823062	-0.20177	-1.39355
C	-2.16494	-1.05086	0.232951
C	2.154847	1.391701	0.653438
C	-1.58256	0.215487	0.461058
C	-3.71201	1.263862	-0.15682
C	-2.3617	1.35717	0.225744

C	3.033094	-1.02501	-2.49785
H	2.266243	-1.72642	-2.81883
C	-4.29044	0.000865	-0.343
C	-3.50148	-1.14748	-0.15329
C	3.81171	0.724352	-1.02238
C	1.551298	-1.72026	0.83731
C	1.325111	-1.69663	2.217994
H	0.954601	-0.7939	2.687863
C	1.684396	2.172062	1.705145
H	0.683426	2.014695	2.082557
C	3.441862	1.59459	0.118271
C	1.990836	-2.89647	0.226406
H	2.181998	-2.92698	-0.83949
C	4.228084	-0.95309	-3.22006
H	4.384988	-1.59676	-4.08032
C	2.503855	3.16718	2.242547
H	2.140245	3.784312	3.058213
C	3.785534	3.368781	1.72709
H	4.423112	4.14174	2.146119
C	5.217493	-0.04922	-2.82987
H	6.14881	0.008608	-3.38527
C	5.011921	0.793916	-1.73729
H	5.783094	1.504209	-1.45653
C	4.255577	2.589254	0.670134
H	5.252796	2.76221	0.27865
C	2.198668	-4.04603	0.989527
H	2.533096	-4.95909	0.506038
C	1.552804	-2.84003	2.980756
H	1.383493	-2.81304	4.053006
C	1.984851	-4.01807	2.367804
H	2.154446	-4.91073	2.962752
O	0.106315	-0.15883	-1.55242
H	0.622319	-0.0033	-2.35585
H	-1.83132	-2.92708	0.197553

TS2 in **4**

E at B3LYP/6-31G** = -5223.87633707 Hartree

Imaginary frequency: 231.5 *i*cm^{-1}

E at B3LYP/SDD + 6-31G**//B3LYP/6-31G** = -2996.23071945 Hartree

Atom	X	Y	Z
As	1.26154	-0.10698	-0.17779
Cl	-5.9635	-0.15856	-0.80692
Cl	-4.15484	-2.76031	-0.40761
Cl	-1.56923	2.902417	0.392442
Cl	-4.65556	2.71004	-0.4083
O	-0.33187	0.299924	0.903691
O	-1.34071	-2.11418	0.390586
C	2.823062	-0.20177	-1.39355
C	-2.16494	-1.05086	0.232951
C	2.154847	1.391701	0.653438
C	-1.58256	0.215487	0.461058
C	-3.71201	1.263862	-0.15682
C	-2.3617	1.35717	0.225744
C	3.033094	-1.02501	-2.49785
H	2.266243	-1.72642	-2.81883
C	-4.29044	0.000865	-0.343
C	-3.50148	-1.14748	-0.15329
C	3.81171	0.724352	-1.02238
C	1.551298	-1.72026	0.83731
C	1.325111	-1.69663	2.217994
H	0.954601	-0.7939	2.687863
C	1.684396	2.172062	1.705145
H	0.683426	2.014695	2.082557
C	3.441862	1.59459	0.118271
C	1.990836	-2.89647	0.226406
H	2.181998	-2.92698	-0.83949
C	4.228084	-0.95309	-3.22006
H	4.384988	-1.59676	-4.08032
C	2.503855	3.16718	2.242547
H	2.140245	3.784312	3.058213
C	3.785534	3.368781	1.72709

H	4.423112	4.14174	2.146119
C	5.217493	-0.04922	-2.82987
H	6.14881	0.008608	-3.38527
C	5.011921	0.793916	-1.73729
H	5.783094	1.504209	-1.45653
C	4.255577	2.589254	0.670134
H	5.252796	2.76221	0.27865
C	2.198668	-4.04603	0.989527
H	2.533096	-4.95909	0.506038
C	1.552804	-2.84003	2.980756
H	1.383493	-2.81304	4.053006
C	1.984851	-4.01807	2.367804
H	2.154446	-4.91073	2.962752
O	0.106315	-0.15883	-1.55242
H	0.622319	-0.0033	-2.35585
H	-1.83132	-2.92708	0.197553

OH-adduct isomer in **4**

E at B3LYP/6-31G** = -5223.89805962 Hartree

E at B3LYP/SDD + 6-31G**//B3LYP/6-31G** = -2996.25339016 Hartree

Atom	X	Y	Z
As	1.537741	-0.39089	-0.50808
Cl	-5.57599	-0.21958	0.386433
Cl	-4.24315	-2.08518	-1.83844
Cl	-0.94231	2.710229	0.514655
Cl	-3.89982	2.206379	1.567162
O	-0.04047	0.705317	-1.46546
O	-1.46024	-1.27956	-2.53329
C	3.139482	-1.29263	0.120017
C	-2.07488	-0.49296	-1.60041
C	2.596053	1.203033	-0.66919
C	-1.28454	0.556948	-1.06802
C	-3.21029	1.170734	0.343829
C	-1.90233	1.395963	-0.11626
C	3.275703	-2.61761	0.51256

H	2.429319	-3.2964	0.463929
C	-3.95641	0.101716	-0.17216
C	-3.37417	-0.71674	-1.15471
C	4.228384	-0.41274	0.196539
C	0.372926	-0.75585	0.966183
C	0.346291	0.049613	2.103683
H	0.980525	0.927501	2.170705
C	2.193009	2.459664	-1.10735
H	1.170195	2.609964	-1.42169
C	3.923038	0.968226	-0.24653
C	-0.45385	-1.87811	0.859254
H	-0.42245	-2.48533	-0.04013
C	4.51023	-3.08124	0.97379
H	4.625698	-4.11757	1.276693
C	3.117581	3.506279	-1.13408
H	2.8101	4.488692	-1.47804
C	4.430947	3.286625	-0.7165
H	5.148944	4.101407	-0.73505
C	5.597723	-2.20686	1.047972
H	6.556662	-2.56614	1.409563
C	5.463828	-0.87213	0.663539
H	6.317032	-0.20445	0.730896
C	4.835572	2.026059	-0.27494
H	5.860566	1.871365	0.045775
C	-1.33613	-2.17841	1.896317
H	-1.99736	-3.03515	1.810589
C	-0.53461	-0.26105	3.139641
H	-0.57299	0.37145	4.020873
C	-1.37874	-1.36827	3.033013
H	-2.07541	-1.59608	3.833826
O	1.264412	-1.53642	-1.817
H	0.462905	-1.22975	-2.28507
H	-2.05633	-1.99783	-2.79406

TS3 in **4**

E at B3LYP/6-31G** = -5223.88859656 Hartree

Imaginary frequency: 886.8 *i*cm^{-1}

E at B3LYP/SDD + 6-31G**//B3LYP/6-31G** = -2996.25056486 Hartree

Atom	X	Y	Z
As	1.765921	0.538857	0.368114
Cl	-5.48866	0.399937	-0.80706
Cl	-4.32558	2.502115	1.296828
Cl	-1.16069	-2.80865	0.198006
Cl	-3.89155	-2.29608	-1.3285
O	-0.35586	-0.58463	1.960543
O	-1.74251	1.640263	2.519196
C	3.349115	1.40033	-0.23116
C	-2.29095	0.760018	1.641766
C	2.718715	-1.0897	0.580613
C	-1.52431	-0.4128	1.388931
C	-3.29533	-1.12646	-0.17555
C	-2.08432	-1.35505	0.499651
C	3.532967	2.719964	-0.62071
H	2.715145	3.432095	-0.57047
C	-4.00811	0.056113	0.052154
C	-3.4929	0.983428	0.974565
C	4.400069	0.462366	-0.29719
C	0.430693	0.493243	-0.98356
C	0.372285	-0.53377	-1.92721
H	1.103632	-1.33551	-1.91296
C	2.256925	-2.30212	1.076307
H	1.235104	-2.38741	1.427
C	4.052706	-0.90881	0.155426
C	-0.53238	1.508611	-0.95996
H	-0.49731	2.260151	-0.17697
C	4.789471	3.13096	-1.07212
H	4.948539	4.161969	-1.37121
C	3.14375	-3.38125	1.132559
H	2.805928	-4.33753	1.518819
C	4.461696	-3.22786	0.696389
H	5.144984	-4.07076	0.740119

C	5.838688	2.21137	-1.1388
H	6.813838	2.531829	-1.49276
C	5.651212	0.881826	-0.75605
H	6.478444	0.182176	-0.81662
C	4.922411	-1.9998	0.214591
H	5.954655	-1.90059	-0.10527
C	-1.56455	1.492244	-1.89583
H	-2.33294	2.25771	-1.86585
C	-0.66531	-0.54323	-2.85848
H	-0.7366	-1.35237	-3.5778
C	-1.63069	0.465773	-2.84051
H	-2.4527	0.438061	-3.54864
O	1.133111	1.291788	1.760031
H	0.332086	0.483885	2.040152
H	-2.32715	2.407833	2.603856

Oxide product in **4**

E at B3LYP/6-31G** = -5223.89446384 Hartree

E at B3LYP/SDD + 6-31G**//B3LYP/6-31G** = -2996.25801639 Hartree

Atom	X	Y	Z
As	1.716381	-0.61845	-0.32553
Cl	-5.17657	0.390587	1.286489
Cl	-3.18263	2.865727	1.069057
Cl	-2.15157	-2.21813	-2.46256
Cl	-4.65065	-2.17976	-0.49799
O	-0.49367	0.261181	-2.32176
O	-0.92314	2.390397	-0.81002
C	3.312241	-1.29956	0.470797
C	-1.83011	1.385501	-0.73906
C	2.654866	0.974694	-0.81544
C	-1.58228	0.250392	-1.53828
C	-3.59099	-0.79873	-0.60604
C	-2.47985	-0.82667	-1.46882
C	3.511133	-2.5135	1.114067
H	2.708499	-3.24179	1.179942

C	-3.82971	0.334385	0.181822
C	-2.95116	1.424676	0.092131
C	4.342515	-0.34322	0.37912
C	0.445839	-0.25157	1.056717
C	0.501296	0.905124	1.837877
H	1.279744	1.642868	1.667026
C	2.183725	2.077928	-1.51763
H	1.164142	2.0952	-1.88379
C	3.980512	0.907828	-0.33465
C	-0.56646	-1.19718	1.248422
H	-0.61117	-2.06361	0.595106
C	4.762092	-2.79954	1.666505
H	4.932308	-3.74896	2.16425
C	3.052563	3.148523	-1.74881
H	2.705459	4.015856	-2.30173
C	4.364725	3.102075	-1.27253
H	5.034607	3.937453	-1.45399
C	5.79203	-1.86	1.5776
H	6.76326	-2.08272	2.009163
C	5.589564	-0.63541	0.938648
H	6.401878	0.081988	0.88098
C	4.832936	1.989857	-0.56969
H	5.857865	1.97185	-0.21315
C	-1.52967	-0.98405	2.233689
H	-2.33105	-1.70284	2.371374
C	-0.46634	1.113945	2.820525
H	-0.44091	2.016706	3.423026
C	-1.4788	0.170999	3.017017
H	-2.24231	0.347146	3.768213
O	1.025323	-1.60066	-1.4906
H	-1.16564	3.073547	-0.1667
H	0.054585	-0.5934	-2.17717

Hydrolysis of **10**

10

E at B3LYP/SDD + 6-31G** = -2920.24305198 Hartree

Atom	X	Y	Z
Cl	-5.58867	-1.30241	-0.09073
Cl	-2.88907	-3.01045	0.120102
Cl	-2.52877	3.224429	-0.68014
Cl	-5.40698	1.837775	-0.49536
O	-0.2998	1.265624	-0.45629
O	-0.45027	-1.31852	-0.13065
C	2.246856	-1.61889	-1.08897
C	-1.61284	-0.66006	-0.20125
C	2.474999	1.627116	-0.52442
C	-1.53545	0.737475	-0.38049
C	-3.95668	0.876119	-0.38293
C	-2.69616	1.502163	-0.46922
C	1.571595	-2.50009	-1.94141
H	0.501583	-2.40386	-2.08507
C	-4.03683	-0.51466	-0.20362
C	-2.85818	-1.28152	-0.11121
C	3.621887	-1.77638	-0.86269
H	4.156945	-1.1062	-0.19458
C	1.446927	-0.27185	2.04263
C	2.385581	0.505607	2.733955
H	2.993676	1.236231	2.208818
C	2.195811	2.857782	0.091063
H	1.350952	2.953007	0.765812
C	3.534331	1.537087	-1.43507
H	3.748371	0.603462	-1.94527
C	0.659098	-1.20812	2.726613
H	-0.06387	-1.80896	2.184459
C	2.277836	-3.52259	-2.5789
H	1.753124	-4.20406	-3.24203
C	2.987848	3.973647	-0.18147
H	2.766378	4.921978	0.299543
C	4.053604	3.874175	-1.07936
H	4.666861	4.744789	-1.29347

C	3.648007	-3.67573	-2.35851
H	4.191502	-4.47535	-2.85342
C	4.31945	-2.80696	-1.49581
H	5.382915	-2.93066	-1.31322
C	4.321983	2.658846	-1.70956
H	5.139818	2.581523	-2.42033
C	0.812987	-1.35863	4.105656
H	0.201614	-2.08052	4.638975
C	2.533499	0.345523	4.113139
H	3.259098	0.948257	4.651465
C	1.747357	-0.58401	4.797246
H	1.862464	-0.70439	5.870624
Sb	1.220731	-0.05661	-0.05344

H_2O

E at B3LYP/SDD + 6-31G** = -76.4181679635 Hartree

Atom	X	Y	Z
O	0	0	0.118882
H	0	0.760245	-0.47553
H	0	-0.76025	-0.47553

H_2O-adduct in **10**

E at B3LYP/SDD + 6-31G** = -2996.68733415 Hartree

Atom	X	Y	Z
Cl	-5.53372	-1.52992	-0.27529
Cl	-2.75513	-3.11871	-0.27164
Cl	-2.69427	3.174966	-0.37253
Cl	-5.50185	1.641395	-0.32603
O	-0.3745	1.314637	-0.37583
O	-0.40222	-1.31192	-0.33375
C	2.472797	-1.66851	-0.60646
C	-1.59178	-0.68947	-0.32312
C	2.446411	1.644511	-0.58958
C	-1.5753	0.72496	-0.34156

C	-4.0072	0.743116	-0.32251
C	-2.77813	1.432947	-0.34155
C	2.001638	-2.77307	-1.32483
H	0.962471	-2.81994	-1.63041
C	-4.02197	-0.66095	-0.30106
C	-2.80624	-1.37438	-0.29949
C	3.803925	-1.64128	-0.16988
H	4.184734	-0.79421	0.395898
C	1.171684	-0.05342	2.050468
C	1.951601	0.836741	2.800277
H	2.586388	1.566591	2.305818
C	2.135682	2.914347	-0.08086
H	1.260905	3.051784	0.546427
C	3.544368	1.486936	-1.44342
H	3.777526	0.513817	-1.86411
C	0.355099	-0.98845	2.701872
H	-0.24503	-1.6837	2.122766
C	2.86282	-3.83281	-1.61735
H	2.49206	-4.6888	-2.17397
C	2.936574	4.010793	-0.40678
H	2.693163	4.992357	-0.01036
C	4.039519	3.847738	-1.24814
H	4.659478	4.702734	-1.50251
C	4.192319	-3.79767	-1.19153
H	4.8587	-4.62423	-1.42093
C	4.66239	-2.70321	-0.4639
H	5.693575	-2.67465	-0.12369
C	4.339416	2.588249	-1.77039
H	5.188419	2.461743	-2.43614
C	0.317319	-1.02489	4.096729
H	-0.3193	-1.74705	4.599586
C	1.912363	0.792214	4.195717
H	2.51753	1.483561	4.775199
C	1.094253	-0.13583	4.842898
H	1.062246	-0.16645	5.928268
O	0.7575	0.055503	-2.60126

H	0.068049	-0.61104	-2.73667
H	0.291962	0.907061	-2.59883
Sb	1.213884	-0.02468	-0.07039

TS1 in **10**

E at B3LYP/SDD + 6-31G** = -2996.66367492 Hartree

Imaginary frequency: 800.0 *i*cm^{-1}

Atom	X	Y	Z
Sb	1.363893	0.064731	-0.29013
Cl	-5.49597	-1.4982	-0.35621
Cl	-2.82022	-3.15144	-0.9286
Cl	-2.46855	3.079263	-0.14789
Cl	-5.31513	1.6411	0.029276
O	-0.28087	1.219648	-0.79937
O	-0.39691	-1.43307	-1.05402
C	2.697398	-1.62435	-0.18922
C	-1.56472	-0.76774	-0.85738
C	2.634264	1.745873	-0.49692
C	-1.4769	0.633235	-0.70124
C	-3.87918	0.712266	-0.30819
C	-2.63635	1.361314	-0.40451
C	2.38163	-2.85605	-0.77929
H	1.443413	-2.98958	-1.30765
C	-3.96039	-0.68198	-0.47464
C	-2.79119	-1.41982	-0.73843
C	3.882216	-1.50029	0.551282
H	4.134131	-0.56197	1.038777
C	0.630873	-0.01414	1.726918
C	-0.14764	1.03358	2.238518
H	-0.40078	1.885602	1.616895
C	2.12032	3.025634	-0.244
H	1.078578	3.152288	0.030311
C	3.966087	1.597901	-0.90539
H	4.372878	0.614647	-1.1226
C	0.914142	-1.12478	2.530333

H	1.500302	-1.95182	2.141806
C	3.254923	-3.93919	-0.65077
H	3.000334	-4.8915	-1.10696
C	2.943864	4.14419	-0.38139
H	2.542143	5.134272	-0.18681
C	4.275021	3.993078	-0.77547
H	4.912502	4.866125	-0.88163
C	4.443321	-3.80331	0.069182
H	5.12005	-4.64721	0.166541
C	4.754716	-2.5844	0.674269
H	5.672416	-2.47637	1.245274
C	4.784677	2.72103	-1.04155
H	5.816294	2.601402	-1.35972
C	0.431361	-1.18254	3.839885
H	0.649567	-2.04938	4.457106
C	-0.62554	0.972696	3.548262
H	-1.23192	1.785586	3.93709
C	-0.33626	-0.13402	4.349412
H	-0.71462	-0.18218	5.366523
O	1.173102	-0.36983	-2.41274
H	1.891813	-0.92762	-2.7447
H	0.209454	-1.04902	-1.98458

OH-adduct in **10**

E at B3LYP/SDD + 6-31G** = -2996.66386130 Hartree

Atom	X	Y	Z
Sb	1.521998	0.066159	-0.5572
Cl	-5.60091	-1.25585	0.020609
Cl	-3.14775	-3.14169	-0.7805
Cl	-2.20867	3.042754	-0.28847
Cl	-5.12038	1.875513	0.247698
O	-0.26725	1.028335	-1.10344
O	-0.63481	-1.6352	-1.3166
C	3.087733	-1.40637	-0.25295
C	-1.71052	-0.86954	-0.97227

C	2.477422	1.915773	-0.16163
C	-1.46575	0.519729	-0.87093
C	-3.81719	0.81518	-0.21678
C	-2.54061	1.340871	-0.47941
C	3.379929	-2.38082	-1.21605
H	2.823571	-2.40343	-2.1487
C	-4.03631	-0.56746	-0.31285
C	-2.96559	-1.39837	-0.68205
C	3.78452	-1.42423	0.964995
H	3.549259	-0.69909	1.740522
C	0.492251	-0.46749	1.264008
C	-0.21425	0.515796	1.966318
H	-0.24964	1.536906	1.598028
C	1.727358	3.101042	-0.15419
H	0.665736	3.072759	-0.37298
C	3.855787	1.960844	0.089875
H	4.451323	1.052935	0.075237
C	0.502376	-1.784	1.734516
H	1.048854	-2.55382	1.197211
C	4.366976	-3.34149	-0.97658
H	4.581591	-4.09557	-1.72878
C	2.355852	4.316965	0.121535
H	1.771769	5.23277	0.128085
C	3.727014	4.358744	0.382206
H	4.211295	5.307405	0.595926
C	5.072101	-3.33447	0.22774
H	5.84156	-4.07863	0.412479
C	4.779598	-2.3748	1.200312
H	5.319617	-2.37182	2.143026
C	4.476948	3.18141	0.362996
H	5.545142	3.211055	0.55818
C	-0.19361	-2.11739	2.898678
H	-0.18967	-3.14348	3.255566
C	-0.90258	0.18258	3.134452
H	-1.45253	0.949106	3.67262
C	-0.89609	-1.13423	3.598629

H	-1.44072	-1.39489	4.501515
O	1.590164	-0.21456	-2.51949
H	2.51277	-0.35439	-2.77802
H	-0.856	-2.57255	-1.20902

TS2 in **10**

E at B3LYP/SDD + 6-31G** = -2996.66317872 Hartree

Imaginary frequency: 207.0 *i*cm^{-1}

Atom	X	Y	Z
Sb	1.502573	0.036262	-0.52737
Cl	-5.59835	-1.30184	-0.06744
Cl	-3.09742	-3.14139	-0.83588
Cl	-2.25709	3.049134	-0.23591
Cl	-5.16813	1.832688	0.21735
O	-0.27482	1.068522	-1.0331
O	-0.59534	-1.58639	-1.29595
C	3.061232	-1.43298	-0.22258
C	-1.69458	-0.84406	-0.96447
C	2.500886	1.874659	-0.18356
C	-1.47165	0.546455	-0.83889
C	-3.83952	0.798129	-0.2327
C	-2.56582	1.346843	-0.45836
C	3.530042	-2.22564	-1.27774
H	3.080492	-2.1191	-2.25949
C	-4.03655	-0.58643	-0.35396
C	-2.94569	-1.39731	-0.70992
C	3.635087	-1.57542	1.049976
H	3.271143	-0.9818	1.884999
C	0.466188	-0.4346	1.309394
C	-0.1906	0.586868	2.005205
H	-0.18103	1.604109	1.625034
C	1.795629	3.086304	-0.24831
H	0.738464	3.085854	-0.49086
C	3.870753	1.879445	0.116041
H	4.427687	0.948306	0.167052

C	0.412358	-1.74675	1.788849
H	0.920464	-2.54592	1.256414
C	4.56015	-3.14558	-1.06363
H	4.914106	-3.76178	-1.88565
C	2.461902	4.288911	-0.00442
H	1.913376	5.225227	-0.05328
C	3.825163	4.291089	0.29868
H	4.338396	5.22976	0.48766
C	5.134631	-3.2731	0.202484
H	5.937926	-3.98593	0.366553
C	4.673553	-2.48526	1.260083
H	5.116708	-2.58308	2.247242
C	4.529324	3.087033	0.357375
H	5.590292	3.085732	0.590504
C	-0.2951	-2.03772	2.957546
H	-0.34076	-3.06033	3.321379
C	-0.89064	0.295802	3.177612
H	-1.4021	1.091825	3.710926
C	-0.94639	-1.01628	3.65208
H	-1.5006	-1.24347	4.55818
O	1.569162	-0.26628	-2.49553
H	2.322402	0.226515	-2.85317
H	-0.79529	-2.53076	-1.20979

OH-adduct isomer in **10**

E at B3LYP/SDD + 6-31G** = -2996.67843114 Hartree

Atom	X	Y	Z
Cl	-5.6527	-0.85502	0.233314
Cl	-3.62058	-2.87058	-1.1843
Cl	-1.77917	3.011363	-0.00241
Cl	-4.72158	2.127833	0.793159
O	-0.21537	0.87955	-1.3186
O	-1.00485	-1.6131	-1.86461
C	3.33444	-1.28568	-0.04131
C	-1.90694	-0.78884	-1.26616

C	2.377398	1.871616	-0.129
C	-1.44907	0.527331	-1.00367
C	-3.6484	1.003485	0.000957
C	-2.35443	1.406395	-0.3742
C	4.213349	-1.7086	-1.04891
H	3.999437	-1.46771	-2.08491
C	-4.06681	-0.31242	-0.24112
C	-3.17945	-1.19833	-0.87508
C	3.610222	-1.61938	1.292878
H	2.931353	-1.31481	2.085867
C	0.34981	-0.83884	1.030973
C	-0.4001	0.038139	1.82229
H	-0.30569	1.113152	1.69852
C	1.71765	3.017549	-0.59197
H	0.79084	2.918841	-1.14153
C	3.578954	1.988895	0.584315
H	4.107131	1.105935	0.930811
C	0.202157	-2.22232	1.179096
H	0.789741	-2.9062	0.572911
C	5.349843	-2.45207	-0.72269
H	6.023606	-2.78061	-1.50923
C	2.260632	4.276958	-0.33061
H	1.749787	5.164948	-0.69153
C	3.449724	4.396626	0.391457
H	3.86486	5.379617	0.595483
C	5.620679	-2.7754	0.608954
H	6.506221	-3.35289	0.859349
C	4.750095	-2.35921	1.61786
H	4.95406	-2.61302	2.654409
C	4.108034	3.253455	0.848743
H	5.035572	3.343067	1.406735
C	-0.70996	-2.72673	2.108008
H	-0.8341	-3.80033	2.215485
C	-1.30471	-0.47114	2.755765
H	-1.89542	0.210785	3.359917
C	-1.46593	-1.85132	2.891454

H	-2.18306	-2.24542	3.605448
O	1.724089	-0.64974	-2.37086
H	0.867391	-0.41863	-2.76448
H	-1.38369	-2.5018	-1.93927
Sb	1.617379	-0.07492	-0.50482

TS3 in **10**

E at B3LYP/SDD + 6-31G** = -2996.65705251 Hartree

Imaginary frequency: 920.4 *i*cm^{-1}

Atom	X	Y	Z
Cl	-5.43215	-0.79869	0.835212
Cl	-4.19274	-2.62742	-1.46779
Cl	-1.44141	2.843708	-0.08897
Cl	-4.05895	1.987534	1.495111
O	-0.57628	0.881626	-2.08851
O	-1.77228	-1.43363	-2.74843
C	3.401492	-1.57551	0.180563
C	-2.34907	-0.67917	-1.78034
C	2.606634	1.659026	-0.32058
C	-1.69089	0.544679	-1.47668
C	-3.42178	0.968077	0.228813
C	-2.26763	1.353488	-0.47483
C	4.659949	-1.47347	-0.42913
H	4.839897	-0.73728	-1.20783
C	-4.03771	-0.25473	-0.06266
C	-3.48857	-1.06239	-1.07418
C	3.182308	-2.52383	1.188122
H	2.209696	-2.60299	1.66668
C	0.310598	-0.48726	1.055434
C	0.170531	0.481849	2.055211
H	0.861101	1.318187	2.116047
C	1.948959	2.69134	-1.00449
H	1.047868	2.484871	-1.57454
C	3.760993	1.91795	0.431464
H	4.276754	1.115876	0.952768

C	-0.61261	-1.53669	0.946493
H	-0.53569	-2.25919	0.138638
C	5.693612	-2.32202	-0.03033
H	6.66851	-2.24396	-0.50224
C	2.458771	3.988795	-0.92761
H	1.95366	4.793373	-1.45356
C	3.607161	4.252995	-0.17756
H	3.996331	5.265612	-0.1216
C	5.473053	-3.26999	0.97196
H	6.279342	-3.92938	1.279591
C	4.220283	-3.37144	1.580092
H	4.050777	-4.10776	2.360068
C	4.258653	3.220565	0.501191
H	5.152431	3.427181	1.082626
C	-1.67041	-1.6198	1.852502
H	-2.403	-2.41479	1.755871
C	-0.89295	0.392494	2.954819
H	-1.02059	1.154891	3.716713
C	-1.81007	-0.65502	2.852457
H	-2.65263	-0.70477	3.534943
O	1.154877	-0.78532	-2.09407
H	0.20705	-0.01692	-2.24301
H	-2.28409	-2.24744	-2.8638
Sb	1.822807	-0.30047	-0.40362

Oxide product in **10**

E at B3LYP/SDD + 6-31G** = -2996.65832976 Hartree

Atom	X	Y	Z
Cl	-5.28336	-0.88504	0.964113
Cl	-4.12216	-2.65523	-1.42081
Cl	-1.48539	2.896586	-0.16067
Cl	-3.98582	1.948871	1.556859
O	-0.70051	1.012183	-2.25296
O	-1.84518	-1.34822	-2.85293
C	3.377974	-1.58522	0.145655

C	-2.37795	-0.63663	-1.83389
C	2.58563	1.646331	-0.29036
C	-1.76076	0.605533	-1.55257
C	-3.38511	0.958847	0.25373
C	-2.28662	1.388523	-0.51281
C	4.648329	-1.4692	-0.43589
H	4.837683	-0.72656	-1.20642
C	-3.96871	-0.28601	-0.01194
C	-3.45529	-1.07023	-1.05807
C	3.148466	-2.54142	1.143238
H	2.167561	-2.63175	1.602531
C	0.311278	-0.49037	1.026452
C	0.193139	0.480859	2.027677
H	0.882336	1.31984	2.065641
C	1.960551	2.699388	-0.97322
H	1.091196	2.512524	-1.59671
C	3.697239	1.890186	0.527702
H	4.190022	1.074264	1.04994
C	-0.60688	-1.5474	0.956983
H	-0.54681	-2.27822	0.15481
C	5.682202	-2.30974	-0.02041
H	6.666197	-2.21905	-0.47096
C	2.455463	3.997059	-0.83039
H	1.972829	4.815539	-1.35625
C	3.562274	4.243114	-0.01452
H	3.941899	5.255232	0.092967
C	5.450281	-3.26559	0.971681
H	6.256261	-3.91905	1.292718
C	4.185882	-3.38181	1.55248
H	4.007121	-4.12377	2.325195
C	4.183638	3.192132	0.663795
H	5.045335	3.38415	1.296609
C	-1.6336	-1.6367	1.897855
H	-2.35926	-2.44146	1.832221
C	-0.83996	0.388307	2.962225
H	-0.9474	1.152389	3.725814

C	-1.74979	-0.66852	2.897612
H	-2.56693	-0.72433	3.60997
O	1.1116	-0.70954	-2.153
H	-0.01	0.232491	-2.37823
H	-2.30378	-2.19781	-2.92679
Sb	1.799745	-0.3121	-0.47003

Hydrolysis of **12**

12

E at B3LYP/SDD + 6-31G** = -2919.04929810 Hartree

Atom	X	Y	Z
Cl	-2.48709	3.356931	0.080289
Cl	-5.39486	2.083492	-0.30407
Cl	-5.67463	-1.05396	-0.66643
Cl	-3.04118	-2.87171	-0.63918
O	-0.32355	1.327932	0.024287
O	-0.55761	-1.27915	-0.28178
C	2.638742	1.381616	-0.05836
C	2.761594	2.594165	0.616379
C	3.871207	3.410375	0.375072
C	4.842519	3.000771	-0.54069
C	4.713383	1.790952	-1.22492
C	3.604745	0.963925	-0.99739
C	3.369578	-0.32688	-1.71552
C	4.222458	-0.84888	-2.69748
C	3.905045	-2.04534	-3.344
C	2.73552	-2.74323	-3.03287
C	1.87279	-2.24259	-2.05373
C	2.201591	-1.05377	-1.4081
C	1.314663	-0.865	2.095773
C	0.472632	-1.89545	2.53481
C	0.611067	-2.3839	3.834979
C	1.58027	-1.84921	4.68724
C	2.41805	-0.82282	4.245157

C	2.288095	-0.32564	2.947302
C	-1.57218	0.830946	-0.13039
C	-1.69171	-0.56653	-0.29526
C	-2.95412	-1.13926	-0.45601
C	-4.10378	-0.32546	-0.46208
C	-3.98035	1.064343	-0.30074
C	-2.70492	1.641114	-0.13219
H	1.992963	2.912024	1.31509
H	3.973152	4.359936	0.891868
H	5.706648	3.630821	-0.73052
H	5.47979	1.50383	-1.93744
H	5.133185	-0.32671	-2.97151
H	4.577187	-2.43209	-4.1046
H	2.495473	-3.66648	-3.55125
H	0.949438	-2.75514	-1.80312
H	-0.27818	-2.30537	1.867322
H	-0.03962	-3.18119	4.181656
H	1.682373	-2.23259	5.698379
H	3.169982	-0.40739	4.909517
H	2.938811	0.474782	2.606737
Sb	1.116245	-0.10159	0.132655

H_2O-adduct in **12**

E at B3LYP/SDD + 6-31G** = -2995.48687837 Hartree

Atom	X	Y	Z
Cl	-2.7627	3.204759	-0.30662
Cl	-5.56127	1.686333	-0.58139
Cl	-5.61315	-1.48464	-0.56913
Cl	-2.8582	-3.08802	-0.28219
O	-0.46754	1.34787	-0.05134
O	-0.50762	-1.30437	-0.04078
C	2.5041	1.393987	-0.58918
C	2.438417	2.784651	-0.56077
C	3.504552	3.532035	-1.07021
C	4.616777	2.874769	-1.60184

C	4.674248	1.480605	-1.63881
C	3.613662	0.713974	-1.13377
C	3.575596	-0.78224	-1.16478
C	4.596275	-1.58077	-1.7025
C	4.467705	-2.97063	-1.72324
C	3.324396	-3.5905	-1.21307
C	2.299433	-2.81011	-0.66874
C	2.430301	-1.42421	-0.64888
C	1.220936	-0.04148	2.251536
C	0.436306	-0.9505	2.973372
C	0.52749	-0.98705	4.365872
C	1.397724	-0.12264	5.034223
C	2.179875	0.78266	4.313629
C	2.092808	0.826729	2.920791
C	-1.66152	0.750524	-0.16774
C	-1.68867	-0.66434	-0.15846
C	-2.89934	-1.34221	-0.28823
C	-4.10407	-0.62338	-0.41828
C	-4.0795	0.780479	-0.42388
C	-2.85351	1.464336	-0.30076
H	1.556392	3.277386	-0.16275
H	3.465478	4.617129	-1.05836
H	5.44713	3.452292	-1.99791
H	5.548724	1.000239	-2.06575
H	5.495009	-1.12841	-2.10925
H	5.267301	-3.57341	-2.14408
H	3.231944	-4.67223	-1.23954
H	1.399111	-3.27451	-0.27691
H	-0.24105	-1.61936	2.450671
H	-0.08201	-1.68868	4.927879
H	1.465211	-0.15333	6.11793
H	2.85412	1.456208	4.83463
H	2.699337	1.536784	2.364493
O	0.433829	-0.15628	-2.44671
H	1.251198	-0.27754	-2.94855
H	0.015492	-1.02937	-2.42465

Sb	1.074387	0.011715	0.143009

TS1 in **12**

E at B3LYP/SDD + 6-31G** = -2995.46244206 Hartree

Imaginary frequency: 695.5 *i*cm^{-1}

Atom	X	Y	Z
Sb	1.210663	0.048298	-0.25674
Cl	-5.64235	-1.45041	-0.41082
Cl	-2.96181	-3.13452	-0.83948
Cl	-2.59491	3.11212	-0.24424
Cl	-5.45265	1.697682	-0.12194
O	-0.39746	1.239208	-0.74983
O	-0.52533	-1.45488	-0.9414
C	2.823699	-1.35006	-0.25636
C	-1.69121	-0.75847	-0.79733
C	2.738738	1.480413	-0.40771
C	-1.59662	0.646936	-0.68332
C	-4.01282	0.750921	-0.37963
C	-2.76351	1.38946	-0.45307
C	2.786822	-2.74208	-0.21739
H	1.831972	-3.26048	-0.18047
C	-4.09873	-0.64757	-0.50311
C	-2.92608	-1.3989	-0.70181
C	4.047452	-0.64545	-0.32075
C	0.512153	-0.08405	1.762243
C	-0.3175	0.914926	2.289253
H	-0.62534	1.754471	1.674618
C	2.607924	2.863531	-0.49352
H	1.620378	3.314918	-0.51461
C	4.002316	0.848719	-0.39204
C	0.899233	-1.16614	2.561126
H	1.544844	-1.94333	2.163182
C	3.982899	-3.46685	-0.22792
H	3.96457	-4.55218	-0.19753
C	3.75673	3.6564	-0.56306

H	3.671095	4.736414	-0.63422
C	5.015201	3.050723	-0.5422
H	5.910176	3.664035	-0.59366
C	5.20026	-2.7846	-0.28016
H	6.132395	-3.34204	-0.28742
C	5.236439	-1.39016	-0.32775
H	6.198754	-0.89069	-0.3727
C	5.141837	1.663218	-0.45797
H	6.134482	1.225203	-0.44661
C	0.453425	-1.25165	3.881981
H	0.751238	-2.09484	4.498603
C	-0.75878	0.824467	3.610371
H	-1.40518	1.597784	4.015073
C	-0.37634	-0.25831	4.405234
H	-0.72559	-0.32824	5.431423
O	0.992838	-0.40594	-2.36372
H	1.741197	-0.93023	-2.68565
H	0.048754	-1.13632	-1.88689

OH-adduct in **12**

E at B3LYP/SDD + 6-31G** = -2995.47343573 Hartree

Atom	X	Y	Z
Sb	1.218455	-0.22376	-0.13002
Cl	-6.1161	-0.00156	-0.97708
Cl	-4.39414	-2.68406	-0.81868
Cl	-1.74202	2.759282	0.830988
Cl	-4.77165	2.747998	-0.13299
O	-0.53254	0.084387	0.974796
O	-1.62285	-2.23948	0.189648
C	2.953698	-0.02796	-1.41241
C	-2.39317	-1.12713	0.108323
C	2.051932	1.507012	0.763107
C	-1.77954	0.084649	0.49921
C	-3.86802	1.259182	-0.04414
C	-2.53306	1.266293	0.401595

C	3.320194	-0.80048	-2.51537
H	2.713404	-1.65307	-2.81448
C	-4.46588	0.048862	-0.42091
C	-3.71332	-1.13517	-0.34353
C	3.735537	1.079041	-1.02302
C	1.636668	-2.04073	0.882768
C	0.83398	-2.46567	1.949025
H	-0.04224	-1.89198	2.221874
C	1.546825	2.190704	1.866024
H	0.604454	1.879858	2.300603
C	3.267694	1.874018	0.151715
C	2.769323	-2.77795	0.514092
H	3.404298	-2.44771	-0.30186
C	4.475934	-0.49117	-3.24048
H	4.762871	-1.09336	-4.09765
C	2.255627	3.280927	2.37764
H	1.870391	3.827421	3.233188
C	3.458837	3.664352	1.781132
H	4.012427	4.511595	2.175864
C	5.256551	0.599672	-2.8541
H	6.154499	0.848359	-3.41239
C	4.891737	1.381194	-1.75668
H	5.513387	2.228181	-1.4848
C	3.963838	2.970256	0.680738
H	4.903651	3.289465	0.24229
C	3.088842	-3.94993	1.203559
H	3.964218	-4.52394	0.913784
C	1.164061	-3.63471	2.635271
H	0.541946	-3.96554	3.461916
C	2.286981	-4.37781	2.262677
H	2.538153	-5.28811	2.79982
O	-0.00895	-0.27107	-1.67458
H	0.515234	-0.14314	-2.47814
H	-2.10844	-2.99028	-0.18316

TS2 in **12**

E at B3LYP/SDD + 6-31G** = -2995.46821210 Hartree

Imaginary frequency: 359.9 *i*cm^{-1}

Atom	X	Y	Z
Sb	1.263238	0.177835	0.155954
Cl	-6.12612	0.305866	1.014372
Cl	-4.09592	2.768198	1.063324
Cl	-2.0711	-2.83549	-0.90516
Cl	-5.08966	-2.52329	0.014739
O	-0.53732	-0.34414	-0.82497
O	-1.37546	2.07345	0.10255
C	3.11473	0.292126	1.272319
C	-2.26398	1.040671	0.090635
C	2.084089	-1.66138	-0.47345
C	-1.77702	-0.20709	-0.36659
C	-4.01299	-1.15256	0.048789
C	-2.67573	-1.2917	-0.36598
C	3.54688	1.265117	2.172971
H	2.936656	2.144612	2.368815
C	-4.47793	0.092904	0.492915
C	-3.58644	1.177649	0.51202
C	3.901516	-0.85197	1.029376
C	1.513819	1.831297	-1.16696
C	0.604199	2.069043	-2.20561
H	-0.26347	1.431448	-2.31478
C	1.514977	-2.55338	-1.3785
H	0.527843	-2.35381	-1.7763
C	3.365847	-1.86912	0.076672
C	2.642766	2.647352	-1.02155
H	3.362803	2.462336	-0.23132
C	4.773964	1.126924	2.828807
H	5.110503	1.88765	3.527283
C	2.224497	-3.70091	-1.74256
H	1.790267	-4.40966	-2.44118
C	3.491581	-3.93023	-1.20266
H	4.046593	-4.82073	-1.48397

C	5.560602	-0.00016	2.583889
H	6.513473	-0.11778	3.09183
C	5.129457	-0.98435	1.694331
H	5.755193	-1.85579	1.530756
C	4.060425	-3.02569	-0.30484
H	5.049813	-3.22843	0.091524
C	2.853405	3.70804	-1.90657
H	3.728025	4.341325	-1.78921
C	0.82513	3.126269	-3.08818
H	0.120829	3.307857	-3.89496
C	1.945191	3.948302	-2.93792
H	2.110974	4.771668	-3.62695
O	0.142973	0.224637	1.777867
H	0.138364	1.109356	2.167209
H	-1.84114	2.88585	0.352297

OH-adduct isomer in **12**

E at B3LYP/SDD + 6-31G** = -2995.48067973 Hartree

Atom	X	Y	Z
Cl	-5.74573	-0.12597	0.31727
Cl	-4.43126	-2.0793	-1.83716
Cl	-1.04102	2.681168	0.452744
Cl	-4.02419	2.278859	1.470943
O	-0.15672	0.613614	-1.46134
O	-1.61915	-1.37396	-2.50625
C	3.308494	-1.28886	0.21972
C	-2.22467	-0.53944	-1.61127
C	2.607541	1.289723	-0.65938
C	-1.42173	0.505757	-1.09217
C	-3.34576	1.200549	0.281422
C	-2.02518	1.379616	-0.16321
C	3.582732	-2.58993	0.634652
H	2.801389	-3.3451	0.622542
C	-4.11153	0.139302	-0.2233
C	-3.53727	-0.71768	-1.17699

C	4.314021	-0.30271	0.222891
C	0.139523	-0.78293	1.212062
C	0.122561	0.069225	2.320087
H	0.821673	0.896685	2.3971
C	2.176434	2.525538	-1.13427
H	1.145896	2.646656	-1.44436
C	3.938507	1.063746	-0.25053
C	-0.78497	-1.82998	1.109665
H	-0.77847	-2.48391	0.241672
C	4.870767	-2.92867	1.060017
H	5.091987	-3.94283	1.379885
C	3.088386	3.58242	-1.20414
H	2.769706	4.55202	-1.57461
C	4.408943	3.3836	-0.79591
H	5.119702	4.20367	-0.8466
C	5.872695	-1.95578	1.070251
H	6.874434	-2.21323	1.402327
C	5.601075	-0.65116	0.656215
H	6.398845	0.084463	0.673233
C	4.833604	2.140116	-0.32462
H	5.867537	2.016233	-0.02008
C	-1.73837	-2.01159	2.11273
H	-2.46824	-2.81086	2.024928
C	-0.82964	-0.12256	3.323178
H	-0.85306	0.546548	4.177963
C	-1.76281	-1.15554	3.215715
H	-2.51389	-1.28918	3.988483
O	1.112618	-1.84381	-1.75912
H	0.303447	-1.60635	-2.24982
H	-2.2373	-2.07664	-2.75841
Sb	1.442739	-0.4626	-0.42906

TS3 in **12**

E at B3LYP/SDD + 6-31G** = -2995.45234559 Hartree

Imaginary frequency: 970.4 *i*cm^{-1}

Atom	X	Y	Z
Cl	-5.6691	-0.23512	0.853088
Cl	-4.65193	-2.40781	-1.25196
Cl	-1.20061	2.736783	-0.24397
Cl	-3.93405	2.382253	1.322321
O	-0.53918	0.473292	-1.99956
O	-2.05514	-1.68109	-2.53444
C	3.504112	-1.38256	0.310024
C	-2.54035	-0.77442	-1.65101
C	2.711238	1.179066	-0.6021
C	-1.72033	0.362792	-1.42025
C	-3.41613	1.175216	0.173187
C	-2.20488	1.334987	-0.52207
C	3.81682	-2.66579	0.750646
H	3.071453	-3.45541	0.727187
C	-4.18968	0.026753	-0.0334
C	-3.73946	-0.93287	-0.95685
C	4.456865	-0.33767	0.331352
C	0.196683	-0.54625	1.150791
C	0.201961	0.480145	2.10083
H	0.990594	1.227147	2.109195
C	2.249306	2.376612	-1.13968
H	1.227681	2.449423	-1.49649
C	4.04393	1.008599	-0.16734
C	-0.84531	-1.48135	1.110769
H	-0.86916	-2.24634	0.339835
C	5.105723	-2.93848	1.21722
H	5.362399	-3.93741	1.556025
C	3.127216	3.461641	-1.22147
H	2.78672	4.404998	-1.63705
C	4.442629	3.324721	-0.77278
H	5.124572	4.167821	-0.83499
C	6.058638	-1.91862	1.245458
H	7.060264	-2.12506	1.610919
C	5.74111	-0.63142	0.809925
H	6.502433	0.140596	0.84699

C	4.903212	2.111964	-0.25577
H	5.936171	2.034126	0.066963
C	-1.88667	-1.38747	2.034837
H	-2.71047	-2.09289	1.992631
C	-0.84527	0.566122	3.019639
H	-0.86059	1.373291	3.745254
C	-1.88699	-0.36323	2.983888
H	-2.71332	-0.27568	3.682377
O	0.896501	-1.44781	-1.88891
H	0.047423	-0.56077	-2.13307
H	-2.66587	-2.43031	-2.59171
Sb	1.653583	-0.6238	-0.37504

Oxide product in **12**

E at B3LYP/SDD + 6-31G** = -2995.45430390 Hartree

Atom	X	Y	Z
Cl	-5.54741	-0.34596	1.043479
Cl	-4.56489	-2.54078	-1.0526
Cl	-1.33093	2.803241	-0.46464
Cl	-3.9402	2.378272	1.291195
O	-0.70018	0.553018	-2.21877
O	-2.12108	-1.70979	-2.56303
C	3.497657	-1.40773	0.305614
C	-2.58443	-0.81339	-1.66295
C	2.722914	1.162837	-0.5912
C	-1.82839	0.372919	-1.5224
C	-3.43587	1.157028	0.155268
C	-2.28238	1.351262	-0.62577
C	3.805144	-2.69716	0.731256
H	3.065377	-3.49014	0.669212
C	-4.15444	-0.03985	0.0419
C	-3.71983	-1.01175	-0.87424
C	4.444239	-0.35978	0.374006
C	0.224208	-0.46344	1.102613
C	0.258067	0.625823	1.980053

H	1.049618	1.366832	1.911344
C	2.270574	2.379314	-1.09562
H	1.260001	2.465512	-1.4813
C	4.039342	0.994775	-0.10877
C	-0.82033	-1.39444	1.165356
H	-0.86898	-2.2141	0.453686
C	5.080335	-2.97268	1.232734
H	5.331574	-3.9764	1.561648
C	3.137541	3.476015	-1.10546
H	2.800827	4.431727	-1.49544
C	4.438	3.334799	-0.61636
H	5.11278	4.185941	-0.62246
C	6.026927	-1.94934	1.307705
H	7.018458	-2.15764	1.698896
C	5.715629	-0.65648	0.884981
H	6.47233	0.117708	0.956932
C	4.890254	2.108558	-0.12545
H	5.909777	2.029815	0.237521
C	-1.82924	-1.2368	2.116397
H	-2.65187	-1.94416	2.154752
C	-0.75787	0.779238	2.925455
H	-0.74833	1.634585	3.593987
C	-1.79811	-0.14975	2.992772
H	-2.59867	-0.0147	3.713414
O	0.874764	-1.42955	-1.93875
H	-0.17708	-0.33161	-2.31092
H	-2.66076	-2.51299	-2.52919
Sb	1.661481	-0.6559	-0.44258

Adducts of **1** and **4** with a solvent molecule

$CHCl_3$ molecule

E at B3LYP/6-31G** = -1419.28272222 Hartree

Atom	X	Y	Z
C	0.000858	0.001041	0.453391

H	0.000192	-0.00014	1.540226
Cl	1.309729	-1.09643	-0.08355
Cl	-1.60468	-0.58605	-0.08345
Cl	0.294632	1.682117	-0.08362

1 in the presence of one $CHCl_3$ molecule

E at B3LYP/6-31G** = -6567.95487859 Hartree

BSSE-corrected *E* at B3LYP/6-31G** = -6567.943433579302 Hartree

Atom	X	Y	Z
As	1.489953	0.3143	0.103423
Cl	-5.04043	-0.09551	1.785978
Cl	-2.2395	-1.24325	2.835174
Cl	-2.32756	2.475681	-2.25138
Cl	-5.08223	1.781013	-0.77042
O	0.015641	1.137668	-0.92703
O	0.047897	-0.38823	1.100038
C	2.599202	-0.93055	1.146535
C	-1.16375	0.085479	0.750215
C	2.464609	0.214496	-1.60246
C	-1.16849	0.934437	-0.37126
C	-3.57484	1.133521	-0.17561
C	-2.37334	1.454021	-0.83891
C	2.234066	-2.26254	1.359318
H	1.2887	-2.63396	0.98151
C	-3.55916	0.298216	0.953279
C	-2.33673	-0.22761	1.421456
C	3.815717	-0.45554	1.648088
H	4.109478	0.577992	1.491103
C	1.868756	1.974499	0.986477
C	2.548548	3.013211	0.347708
H	2.890278	2.900228	-0.67604
C	2.181535	1.092726	-2.6621
H	1.378294	1.81115	-2.57102
C	3.465526	-0.7527	-1.76096
H	3.685209	-1.45608	-0.96772

C	1.431328	2.120076	2.307325
H	0.909276	1.303873	2.79664
C	3.080291	-3.11279	2.072541
H	2.788915	-4.14571	2.238813
C	2.923108	1.025417	-3.8404
H	2.703631	1.71636	-4.64874
C	3.928689	0.067849	-3.98825
H	4.496798	0.012943	-4.91219
C	4.29244	-2.63625	2.575616
H	4.948246	-3.29848	3.1332
C	4.660084	-1.30677	2.361896
H	5.599867	-0.92981	2.754688
C	4.191649	-0.82537	-2.95081
H	4.961496	-1.58285	-3.06262
C	1.667049	3.315509	2.984154
H	1.321852	3.432956	4.006805
C	2.788468	4.20511	1.032464
H	3.317683	5.013981	0.537838
C	2.34505	4.357511	2.347406
H	2.529111	5.287476	2.87705
C	-1.34521	-2.95744	-1.53398
H	-1.3743	-3.80968	-2.20801
Cl	-2.78136	-1.95145	-1.85654
Cl	0.171559	-2.05879	-1.88285
Cl	-1.34867	-3.58506	0.140817

4 in the presence of one $CHCl_3$ molecule

E at B3LYP/6-31G** = -6566.76019398 Hartree

BSSE-corrected *E* at B3LYP/6-31G** = -6566.749727222899 Hartree

Atom	X	Y	Z
As	-1.32559	-0.49191	0.158229
Cl	2.314114	-1.90968	-2.80586
Cl	5.168482	-1.30516	-1.48233
Cl	5.292603	0.069742	1.372804
Cl	2.559568	0.822843	2.867011

O	0.05291	-1.02254	-1.0468
O	0.152499	0.104713	1.225868
C	-2.55977	-0.44214	-1.34054
C	-2.46528	-1.11377	-2.55589
C	-3.48119	-0.96286	-3.50345
C	-4.57016	-0.13152	-3.23009
C	-4.65162	0.561746	-2.02163
C	-3.63777	0.418525	-1.069
C	-3.5703	1.130757	0.231097
C	-4.52026	2.038888	0.709481
C	-4.31675	2.673203	1.935597
C	-3.17199	2.410969	2.69224
C	-2.22111	1.499971	2.226159
C	-2.43191	0.862156	1.009046
C	-1.65261	-2.14843	1.072367
C	-1.0509	-2.38689	2.313946
C	-1.28332	-3.5874	2.983301
C	-2.11728	-4.55444	2.419396
C	-2.71899	-4.31927	1.182601
C	-2.48764	-3.11957	0.509968
C	1.28442	-0.8401	-0.55882
C	1.341445	-0.216	0.70037
C	2.564139	0.062468	1.298057
C	3.755622	-0.27581	0.624634
C	3.70003	-0.88686	-0.63891
C	2.45303	-1.16879	-1.23445
H	-1.60457	-1.73874	-2.76453
H	-3.41737	-1.48276	-4.45425
H	-5.35776	-0.01281	-3.96832
H	-5.49693	1.21561	-1.83317
H	-5.4117	2.260856	0.131608
H	-5.05443	3.382261	2.299488
H	-3.01671	2.91945	3.638765
H	-1.32003	1.30291	2.794449
H	-0.39902	-1.63984	2.752397
H	-0.81051	-3.76649	3.944151

H	-2.29622	-5.48949	2.941887
H	-3.3663	-5.06893	0.737745
H	-2.95648	-2.9493	-0.45331
C	0.817695	3.195184	-0.9799
H	0.741447	4.178091	-1.43747
Cl	0.589974	3.386082	0.77887
Cl	-0.48443	2.18126	-1.69309
Cl	2.431596	2.535203	-1.369

THF molecule

E at B3LYP/6-31G** = -232.467547330 Hartree

Atom	X	Y	Z
O	0.00002	-1.25248	0
C	-1.16473	-0.42933	0.134257
H	-1.52956	-0.47381	1.172271
H	-1.95328	-0.82159	-0.51831
C	1.164743	-0.42929	-0.13426
H	1.529585	-0.4738	-1.17227
H	1.953307	-0.8215	0.518333
C	-0.73198	0.995568	-0.23185
H	-0.78613	1.14458	-1.3163
H	-1.34525	1.76307	0.248347
C	0.731945	0.995592	0.231838
H	0.786063	1.144552	1.316306
H	1.345209	1.763134	-0.24831

1 in the presence of one THF molecule

E at B3LYP/6-31G** = -5381.15409596 Hartree

BSSE-corrected *E* at B3LYP/6-31G** = -5381.130466199838 Hartree

Atom	X	Y	Z
As	1.114611	-0.16564	0.227586
Cl	-5.41578	-1.22806	-1.03197
Cl	-2.62878	-2.65516	-1.719
Cl	-2.58734	2.90379	1.249566

Cl	-5.39491	1.572642	0.460291
O	-0.26716	1.21488	0.394345
O	-0.27789	-1.0268	-0.8158
C	2.270255	-1.60029	-0.48772
C	-1.48488	-0.51565	-0.54812
C	2.44093	1.224198	0.709732
C	-1.47522	0.720438	0.131268
C	-3.89714	0.764053	0.074966
C	-2.67107	1.362266	0.433679
C	2.324703	-1.91965	-1.84668
H	1.72282	-1.35922	-2.55016
C	-3.90621	-0.47261	-0.58882
C	-2.689	-1.11679	-0.89689
C	3.004992	-2.36751	0.424591
H	2.940256	-2.16743	1.489384
C	0.616727	-0.93161	1.933934
C	0.787307	-0.21301	3.118887
H	1.232241	0.7766	3.100005
C	2.085221	2.572052	0.860552
H	1.055398	2.875522	0.737315
C	3.781933	0.856401	0.874205
H	4.095935	-0.17123	0.742059
C	0.021211	-2.19718	1.957721
H	-0.12352	-2.73907	1.028893
C	3.1352	-2.96389	-2.29263
H	3.166491	-3.20502	-3.35127
C	3.054089	3.525032	1.177947
H	2.760935	4.564666	1.292285
C	4.387485	3.150633	1.348935
H	5.138712	3.895212	1.595363
C	3.892575	-3.7045	-1.38334
H	4.523613	-4.51665	-1.7322
C	3.823136	-3.40702	-0.02256
H	4.393543	-3.98933	0.69517
C	4.747049	1.81199	1.199676
H	5.781118	1.505261	1.327145

C	-0.3833	-2.75149	3.170958
H	-0.84697	-3.73328	3.189057
C	0.383179	-0.77082	4.332235
H	0.518071	-0.21399	5.254803
C	-0.2008	-2.03899	4.35843
H	-0.51835	-2.47002	5.303448
O	1.411085	0.89054	-1.94336
C	0.28608	1.59209	-2.52215
H	-0.08502	2.322	-1.79636
H	-0.49588	0.856526	-2.71652
C	2.658158	1.394289	-2.47862
H	3.107252	0.599668	-3.08621
H	3.331422	1.627282	-1.65296
C	0.848374	2.264544	-3.7698
H	0.87733	1.558928	-4.60741
H	0.260544	3.134388	-4.07351
C	2.273176	2.616197	-3.31368
H	2.257107	3.511082	-2.68211
H	2.967111	2.791549	-4.13953

4 in the presence of one THF molecule

E at B3LYP/6-31G** = -5379.96542897 Hartree

BSSE-corrected *E* at B3LYP/6-31G** = -5379.943236192341 Hartree

Atom	X	Y	Z
As	1.18874	0.294969	0.223599
Cl	-2.60032	2.162255	-2.26758
Cl	-5.37909	1.045608	-1.1222
Cl	-5.34383	-0.93091	1.36075
Cl	-2.53478	-1.74748	2.668452
O	-0.26142	1.198872	-0.67796
O	-0.23469	-0.3717	1.339372
C	2.330122	0.525634	-1.33292
C	2.196141	1.445104	-2.36469
C	3.156837	1.476034	-3.37973
C	4.236792	0.590648	-3.34456

C	4.36773	-0.331	-2.30445
C	3.407712	-0.37506	-1.28787
C	3.413793	-1.30789	-0.13426
C	4.36135	-2.31123	0.095315
C	4.237187	-3.14304	1.209404
C	3.174316	-2.98468	2.102171
C	2.224306	-1.98299	1.882167
C	2.356809	-1.14871	0.779001
C	1.691107	1.779292	1.355906
C	2.722975	1.638716	2.29085
C	3.105781	2.715162	3.091362
C	2.459178	3.944674	2.965646
C	1.430329	4.093035	2.03459
C	1.049975	3.017829	1.232388
C	-1.46012	0.799421	-0.2436
C	-1.44266	-0.06866	0.867384
C	-2.63012	-0.61943	1.340358
C	-3.85571	-0.26954	0.7359
C	-3.87182	0.603732	-0.36381
C	-2.66076	1.125824	-0.86456
H	1.347521	2.119663	-2.38645
H	3.061996	2.186265	-4.19557
H	4.983188	0.616654	-4.13302
H	5.214914	-1.00966	-2.29343
H	5.189675	-2.45413	-0.59139
H	4.973691	-3.92306	1.378802
H	3.081578	-3.64226	2.96111
H	1.385634	-1.85914	2.558139
H	3.231184	0.687701	2.408501
H	3.906499	2.589501	3.814192
H	2.754654	4.782559	3.590337
H	0.921643	5.046892	1.930453
H	0.252925	3.145327	0.509609
O	0.368043	-1.53179	-1.20113
C	-0.10439	-2.78055	-0.63252
H	0.759877	-3.43144	-0.47072

H	-0.55722	-2.55884	0.335772
C	-0.2631	-1.29409	-2.47702
H	-0.38983	-0.21823	-2.59077
H	0.395031	-1.66432	-3.27495
C	-1.56324	-2.08797	-2.40877
H	-2.31155	-1.53237	-1.83553
H	-1.97791	-2.30994	-3.39533
C	-1.11583	-3.34312	-1.64083
H	-1.94021	-3.8626	-1.14611
H	-0.62921	-4.04963	-2.321

Reference

[1] K.Hirose, *J. Incl. Phenom. Macrocycl. Chem.* 2001, **39**, 193.