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Supporting Information

Catalysis with Pnictogen, Chalcogen, and Halogen Bonds

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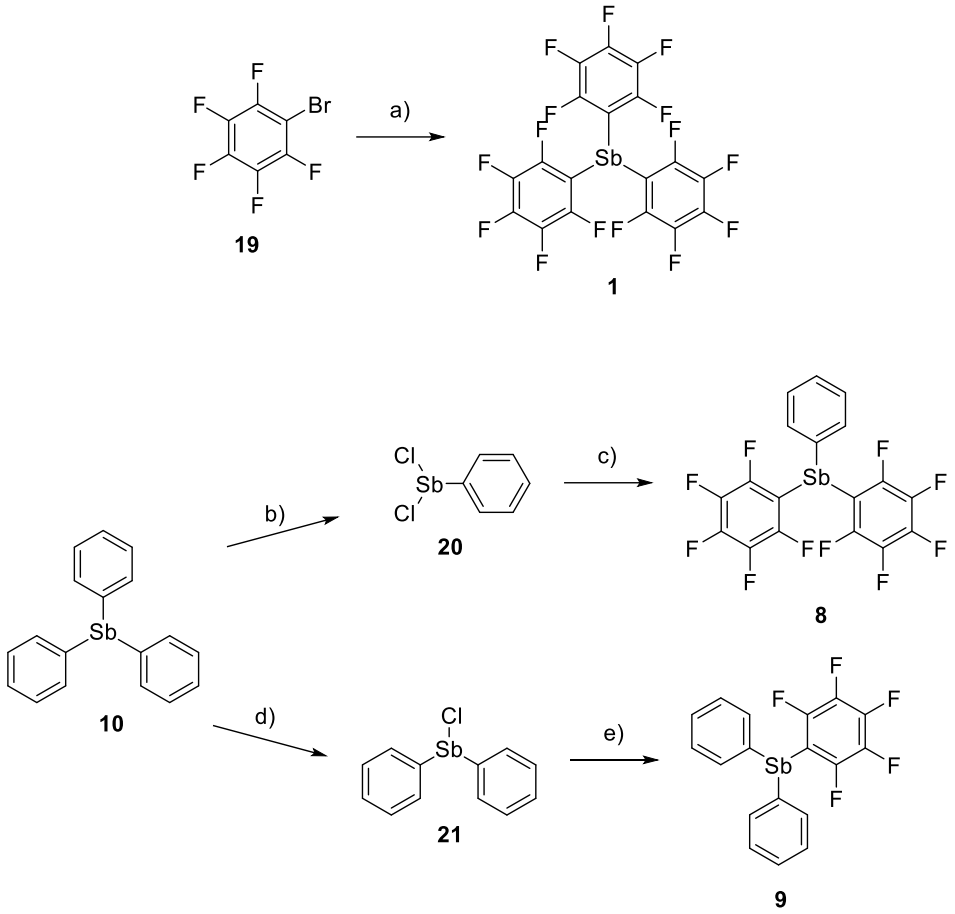
Table of Content

1. Materials and Methods

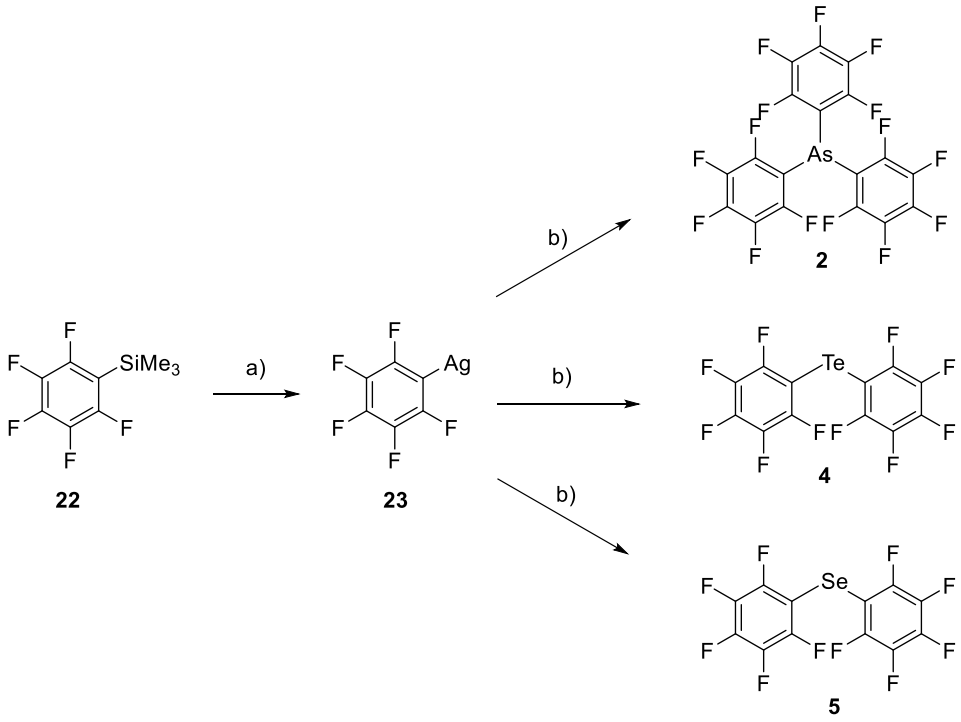
As in reference [S1], supporting information. Reagents for synthesis were purchased from Fluka, Sigma-Aldrich, Apollo Scientific and Acros. Column chromatography was carried out on silica gel (SiliaFlash® P60, SILICYCLE, 230–400 mesh). Analytical (TLC) and preparative thin layer chromatography (PTLC) were performed on silica gel 60 F254 (Merck) and silica gel (SiliCycle, 1000 μm), respectively. ^{1}H NMR spectra were recorded either on a Bruker 300 MHz, 400 MHz or 500 MHz spectrometer. Cryogenic reactions were carried out in a Eyela PSL 2500B Cooling machine.

Abbreviations. BSSE; Basis set superposition error; BuLi: *n*-Butyllithium; NMR: Nuclear magnetic resonance; MEP; Molecular electrostatic potential; rt: Room temperature; TBACl: Tetrabutylammonium chloride; THF: Tetrahydrofuran.

2. Synthesis



Scheme S1. Reagents and conditions: a) 1) BuLi, −78 °C, 15 min; 2) $SbCl_3$, −78 °C to rt, 2 h, 95%; b) 2 eq. $SbCl_3$, neat, 3 d, quant; c) 1) bromopentafluorobenzene, BuLi, THF, −78 °C; 2) **20**, −78 °C to rt, 2 h, 29%; d) 1 eq. $SbCl_3$, neat, 3 d; quant; (e) bromopentafluorobenzene, BuLi, THF, −78 °C. 2) **21**, −78 °C to rt, 2 h, 7%.



Scheme S2. Reagents and conditions: a) EtCN, AgF, rt, 2 h, quant; b) **2**: As, 60 °C, 14 h, 60%, **4**: Te, 60 °C, 48 h, 12%, **5**: Se, 60 °C, 45%.

Compound 1. Was synthesized according to the procedure reported in ref. [S2].

Compound 8. Was synthesized according to the procedure reported in ref. [S2].

Compound 9. Was synthesized according to the procedure reported in ref. [S2].

Compound 2. Was synthesized according to the procedure reported in ref. [S3].

Compound 4. Was synthesized according to the procedure reported in ref. [S3].

Compound 5. Was synthesized according to the procedure reported in ref. [S3].

3. Anion Binding

TBACl was dried by lyophilization. For catalysts **1**, **8** and **9**, 50 μL of a ~ 18 mM stock solution of catalyst in dry THF was injected into an NMR tube and diluted with the appropriate amount of dry THF, then the appropriate amount of stock solution of TBACl in dry THF was added to reach a total volume of 0.5 mL. For catalysts **2-7** a ~ 1.8 mM stock solution was prepared and this stock solution was used to prepare the TBACl stock solution. Various volumes of stock solution with or without TBACl were mixed in an NMR tube to reach the desired final TBACl concentration. Solutions prepared by either method were thoroughly mixed and ^{19}F NMR spectra were recorded. Differences in chemical shift, $\Delta\delta$ of the most responsive fluorine signal, in para position to the heteroatom, were plotted versus TBACl concentration and curve-fitted to a 1:1 binding isotherm in order to determine dissociation constants (K_D's)[S4] according to Equation (S1):

$$\Delta\delta = (\Delta\delta_{max} / [C]_0) \times (0.5 \times [A] + 0.5 \times ([C]_0 + K_D) - (0.5 \times (([A]^2) + (2 \times ([A]) \times (K_D - [C]_0)) + (K_D + [C]_0)^2)^{0.5})) \quad \text{(S1)}$$

where $\Delta\delta = |\delta - \delta_0|$, [A] = concentration of TBACl, and $[C]_0$ = concentration of catalyst **1**, **2**, **4**, **5**, **8** and **9**.

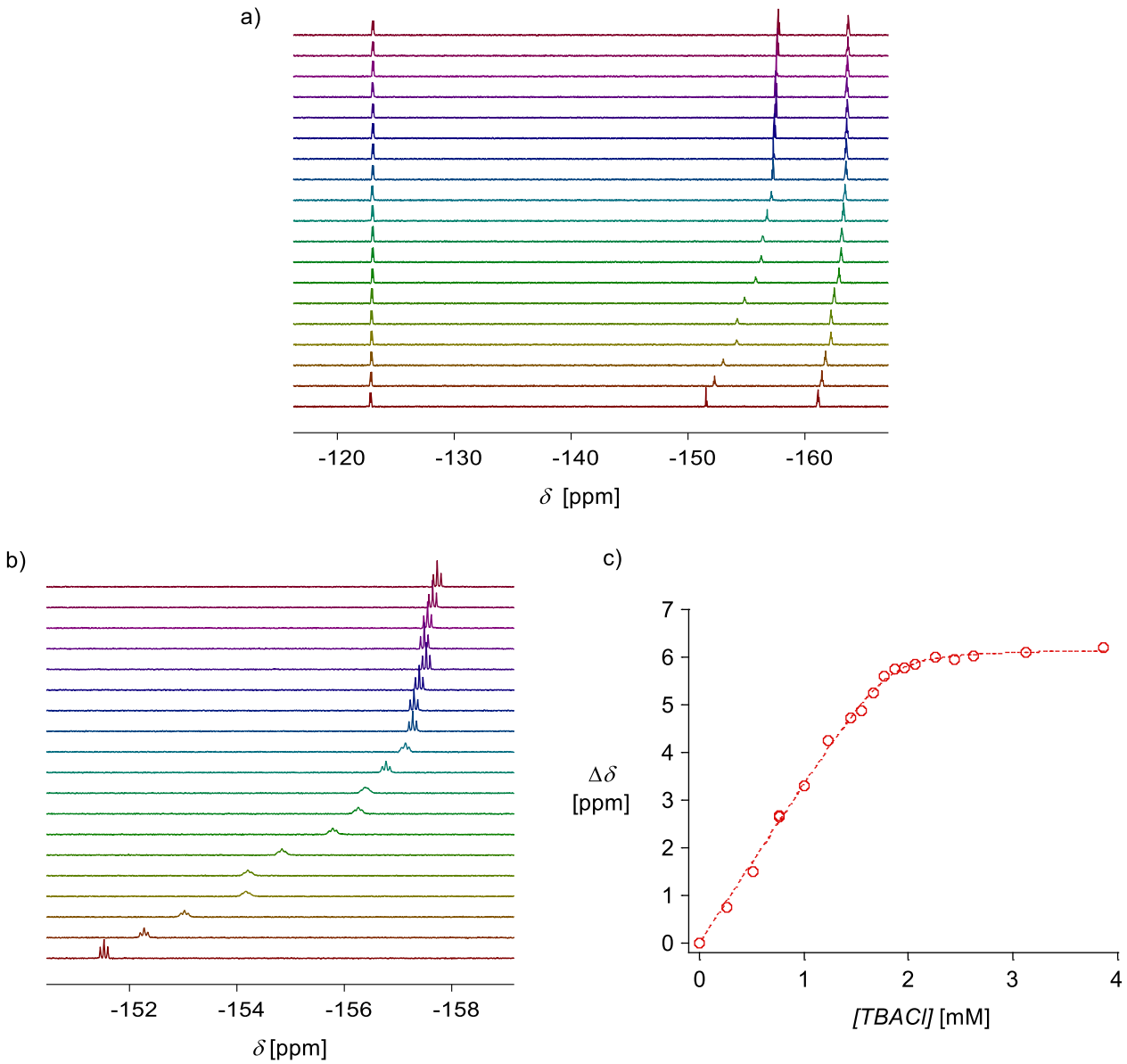


Figure S1. ^{19}F NMR spectra of a) a 1.81 mM THF solution of catalyst **1** with increasing concentration of TBACl (bottom to top) and b) zoom of the most responsive signal. c) Nonlinear fitting according to Equation (S1), of changes in chemical shift $\Delta\delta$ versus TBACl concentration.

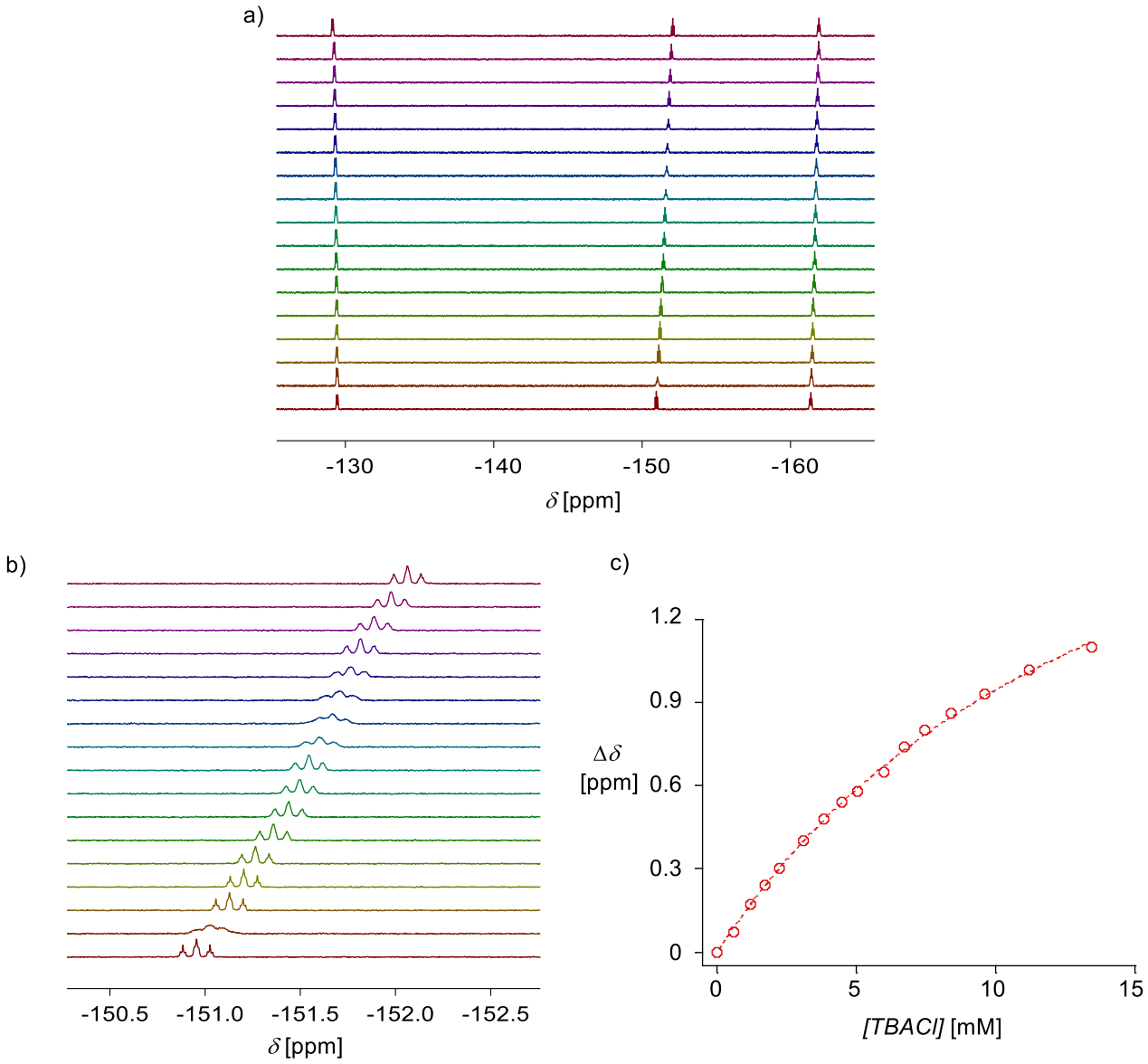


Figure S2. ^{19}F NMR spectra of a) a 1.79 mM THF solution of catalyst **2** with increasing concentration of TBACl (bottom to top) and b) zoom of the most responsive signal. c) Nonlinear fitting according to Equation (S1), of changes in chemical shift $\Delta\delta$ versus TBACl concentration.

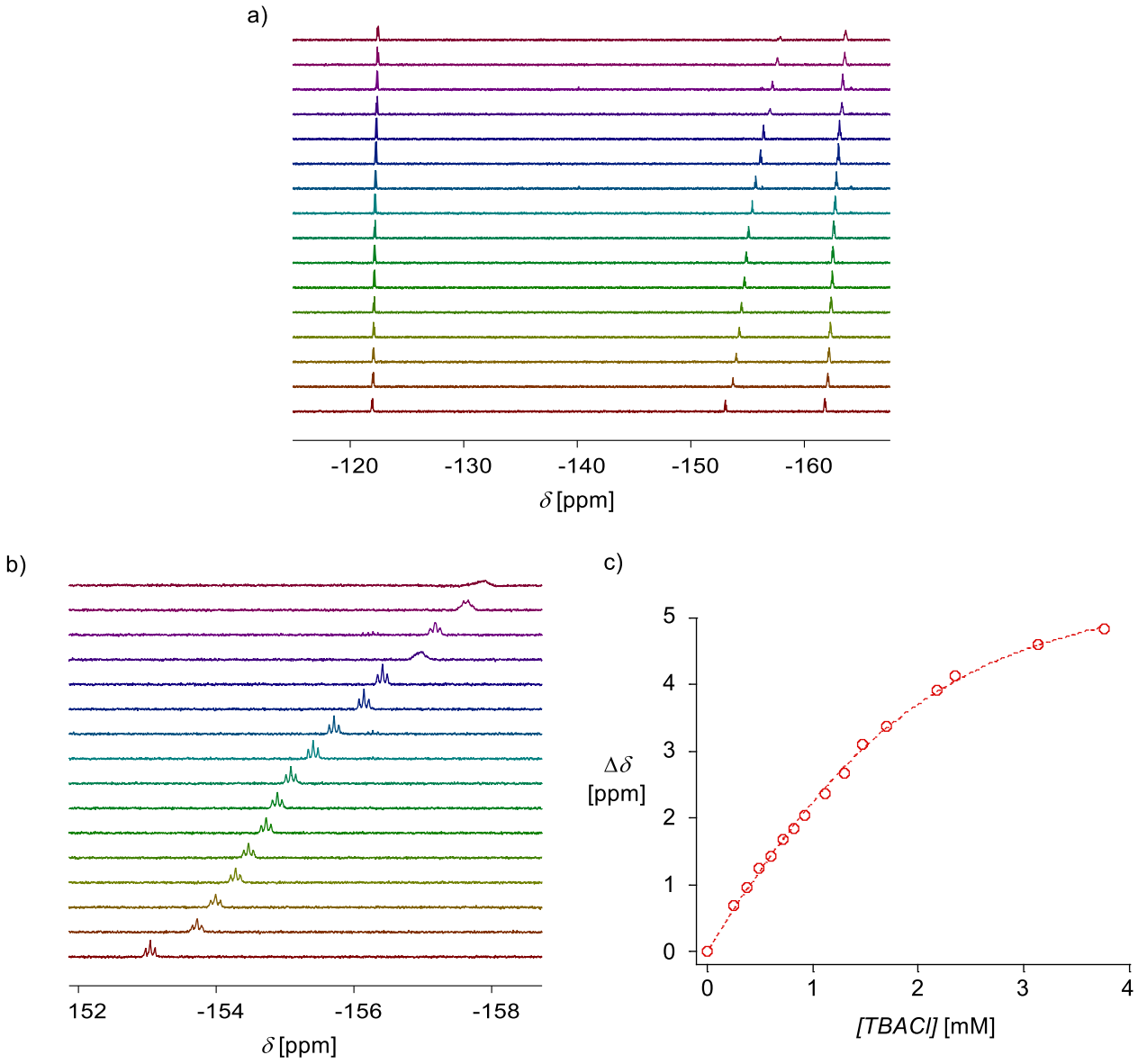


Figure S3. ^{19}F NMR spectra of a) a 1.81 mM THF solution of catalyst **8** with increasing concentration of TBACl (bottom to top) and b) zoom of the most responsive signal. c) Nonlinear fitting according to Equation (S1), of changes in chemical shift $\Delta\delta$ versus TBACl concentration.

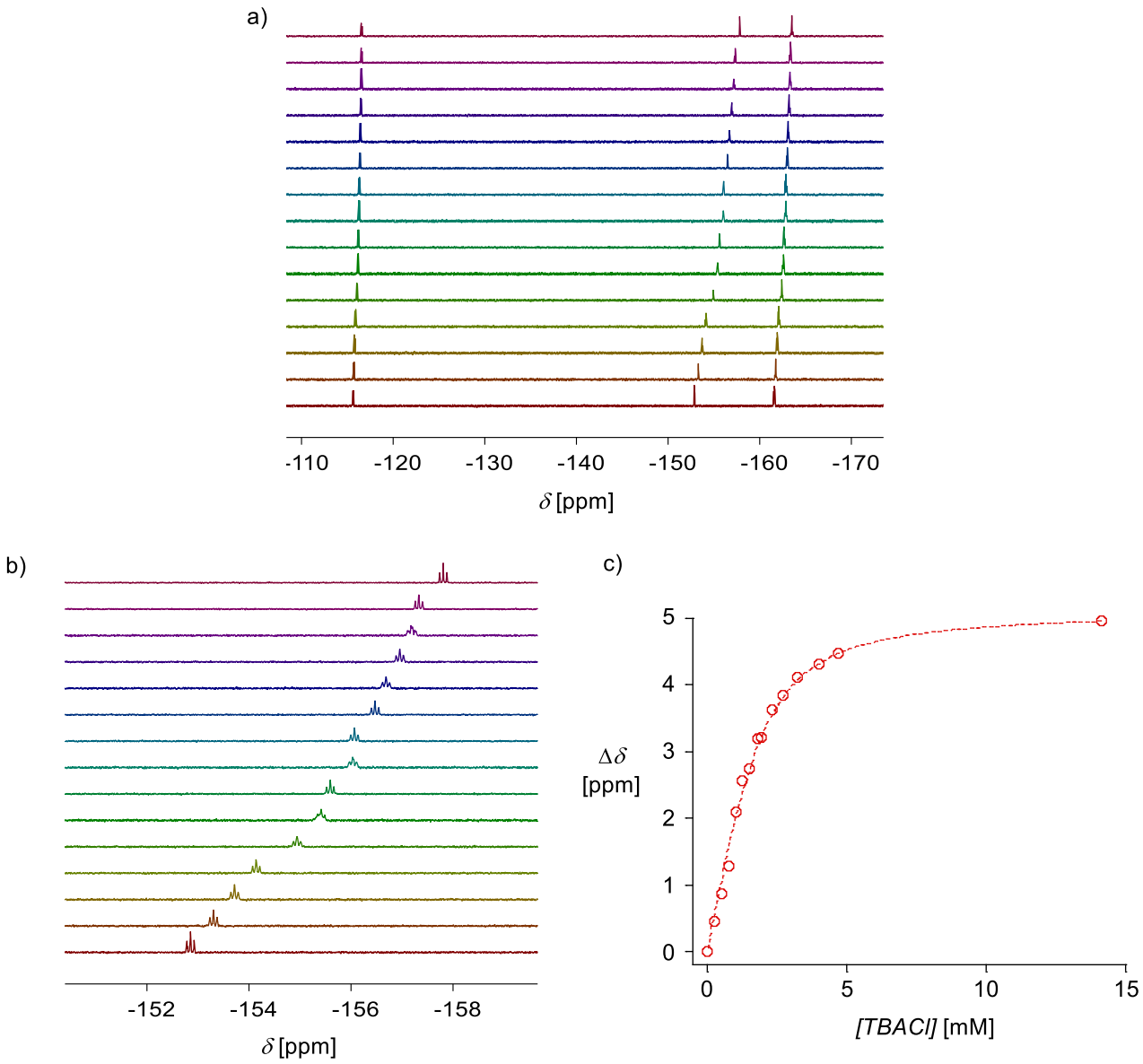


Figure S4. ^{19}F NMR spectra of a) a 1.86 mM THF solution of catalyst **4** with increasing concentration of TBACl (bottom to top) and b) zoom of the most responsive signal. c) Nonlinear fitting according to Equation (S1), of changes in chemical shift $\Delta\delta$ versus TBACl concentration.

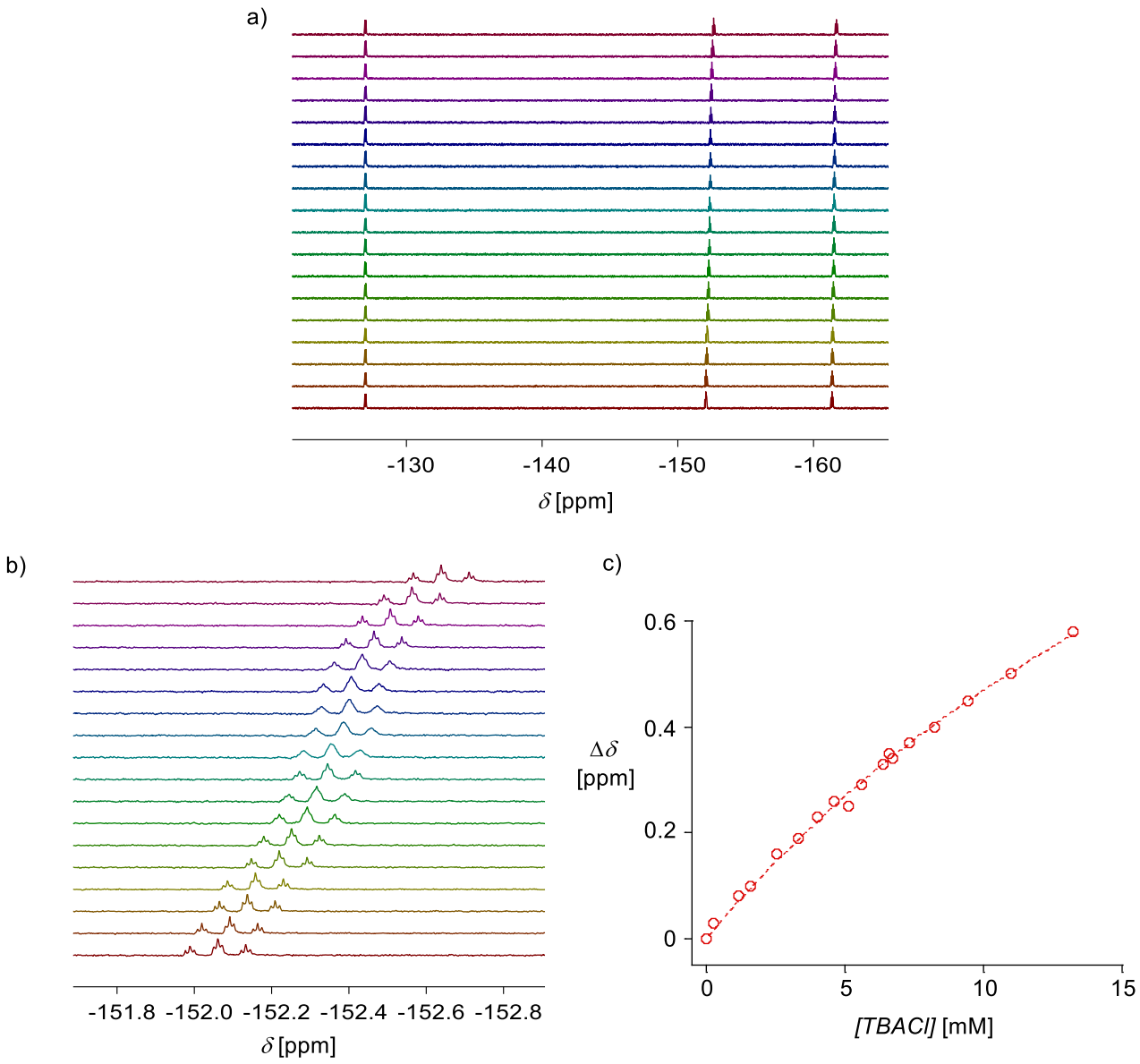


Figure S5. ^{19}F NMR spectra of a) a 1.86 mM THF solution of catalyst **5** with increasing concentration of TBACl (bottom to top) and b) zoom of the most responsive signal. c) Nonlinear fitting according to Equation (S1), of changes in chemical shift $\Delta\delta$ versus TBACl concentration.

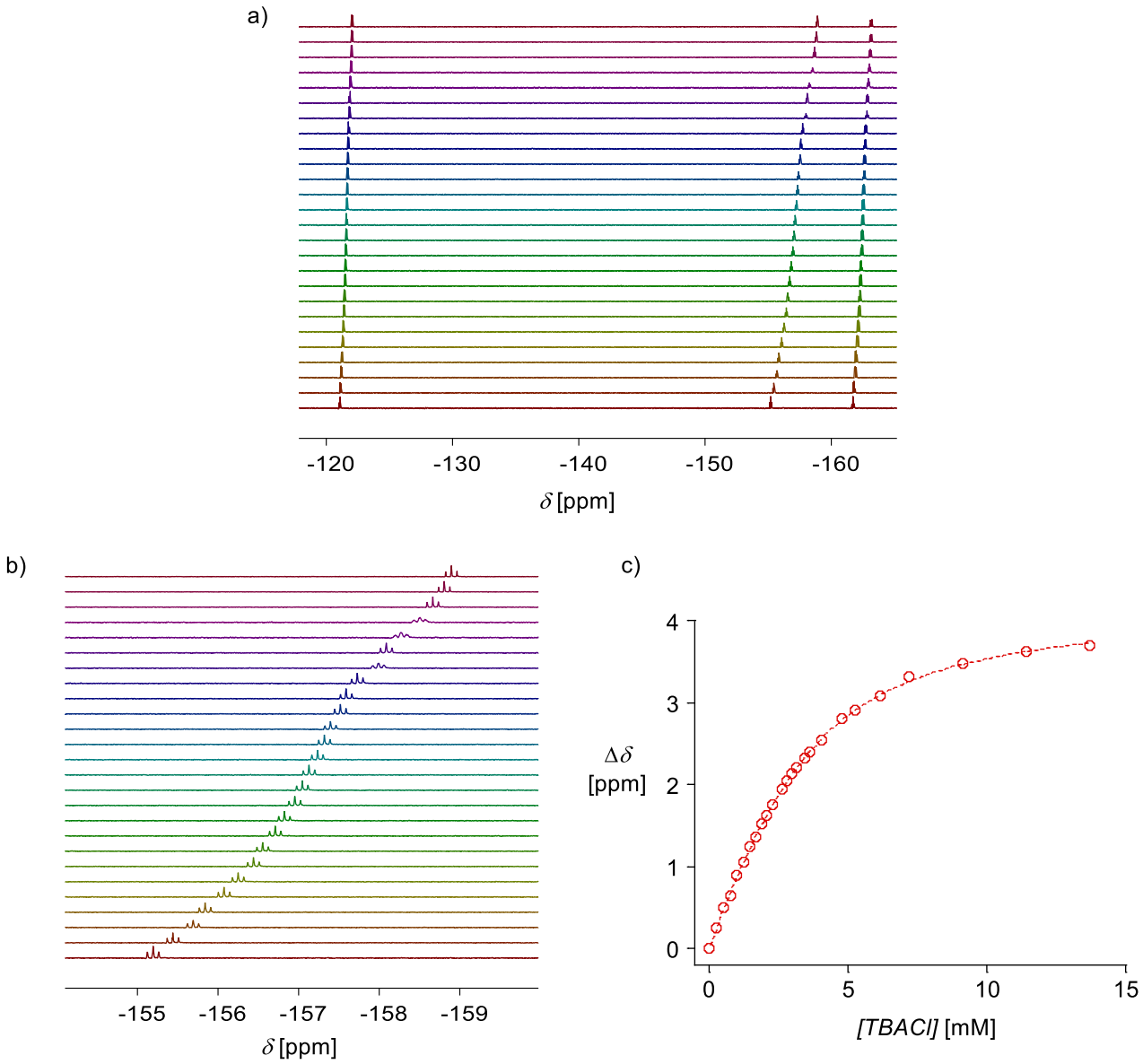


Figure S6. ^{19}F NMR spectra of a) a 3.12 mM THF solution of catalyst **6** with increasing concentration of TBACl (bottom to top) and b) zoom of the most responsive signal. c) Nonlinear fitting according to Equation (S1), of changes in chemical shift $\Delta\delta$ versus TBACl concentration.

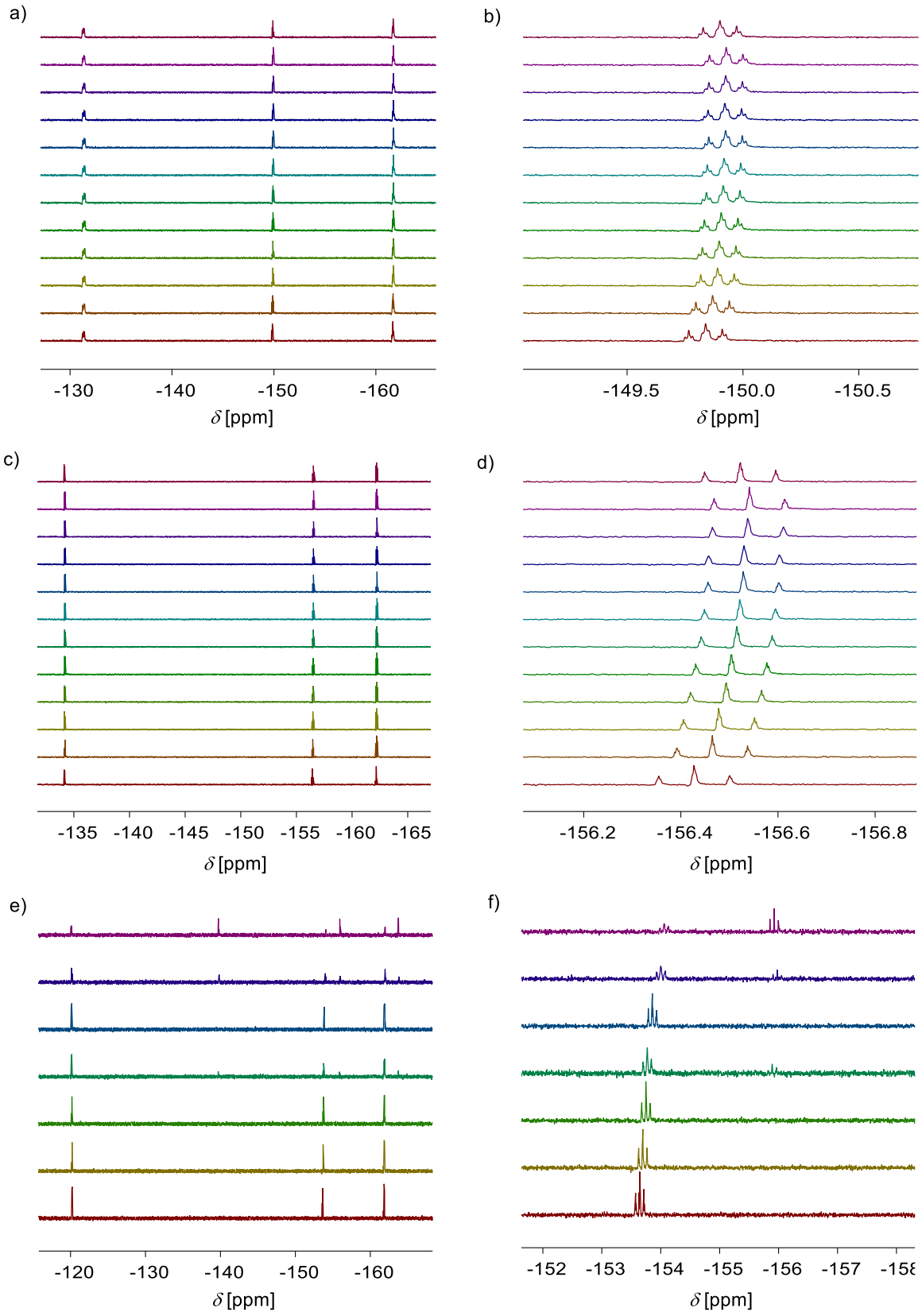
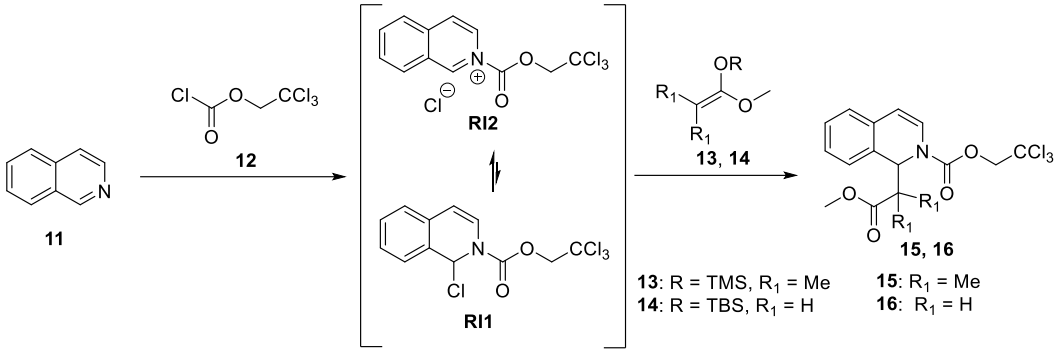


Figure S7. ^{19}F NMR spectra of THF solution of a) catalysts **3**, c) catalyst **7** and e) catalyst **9**. No significant shifts are observed up to a concentration of 15 mM of TBACl b) for catalysts **3**, d)

catalyst **7** and f) catalyst **9**. At higher TBACl concentrations some decomposition of catalyst **9** is observed.

4. Catalyst Evaluation

4.1. Reissert Type Addition to Isoquinolines



Scheme S3. Reactions with substrate **11** (25 mM), **12** (27.5 mM) and nucleophile **13** or **14** (37.5 mM) together with catalysts and 1,4-bis(trimethylsilyl)benzene (6.25 mM) as internal standard were conducted in dry solvent.

Similarly to the previously described procedure in reference [S5], an oven dried microwave vial with a magnetic stir bar freshly taken from the oven was capped with a rubber septum and cooled to rt. A stock solution (1 mL) of substrate **11** (50 mM, 0.05 mmol) and internal standard 1,4-bis(trimethylsilyl)benzene (12.5 mM, 0.0125 mmol) in dry solvent (THF, Toluene or Ether) was injected into the vial. Subsequently acylating agent **12** (7.6 µL, 0.055 mmol) was added and the mixture was stirred for 20 min at rt. Successively the mixture was cooled to -78 °C or -100 °C and a stock solution of catalyst (1 mL) in dry solvent or only dry solvent for blanks was added and stirred for 15 min. Subsequently the nucleophile **13** (15 µL, 0.075 mmol) or **14** (16 µL, 0.075 mmol) was added and stirred for the appropriate amount of time. Reactions were quenched by the addition of 0.2 mL of a 0.5 M solution of NaOMe in methanol and filtered cold through a silica filled pipette,

the product was eluted with EtOAc, the solvent removed in vacuo and the residue was taken up in $CDCl_3$ and analyzed by ^1H NMR spectroscopy.

After baseline correction, the integral associated with the methyl ester protons in product **15** or **16** (two separate signals due to carbamate rotamers as reported in reference [S5] for product **15**: (δ 3.63 ppm; s, and δ 3.61 ppm; s, 3H total) and as reported in reference [S6] for product **16**: (δ 3.63 ppm; s, and δ 3.61 ppm; s, 3H total)) was compared with the integral of the aromatic signal of the internal standard 1,4-bis(trimethylsilyl)benzene at (δ 7.52 ppm; s, 4H) as depicted in Figure S8. The yield η of the product was determined according to Equation (S2).

$$\eta = \frac{\int Product}{\int Standard} \times \frac{1}{3} \qquad \text{(S2)}$$

where the integral ratio of product vs standard is corrected to account for different concentrations and numbers of protons.

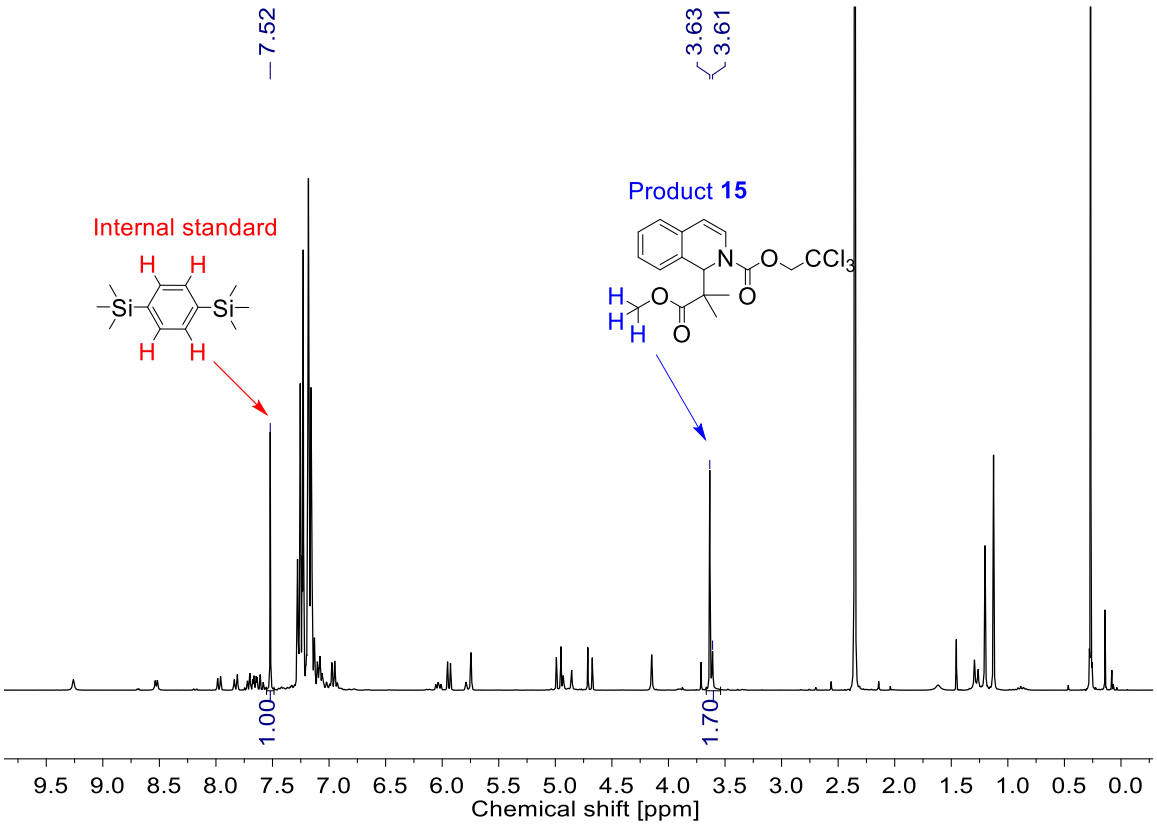


Figure S8. Representative ^1H NMR spectra with integrated signals for the internal standard (red protons/arrow) at δ 7.52 ppm and product **15** (blue arrow/protons) at δ 3.63 ppm / δ 3.61 ppm.

4.1.1. Initial Screening

Following the procedure outlined in section 4.1., catalyst **1** (20 mol%) or blank reactions were employed with the conditions given in Table S1.

Table S1: Initial screening of conditions.

Cat[a]	Nucleophile	Solvent	*T* [°C]	*t* [h]	*η* [%][b]
1	**14**	Toluene	−78	1	57
-	**14**	Toluene	−78	1	18
1	**14**	Toluene	−78	64	74
-	**14**	Toluene	−78	64	27
1	**13**	Toluene	−78	1	60
-	**13**	Toluene	−78	1	5
1	**13**	THF	−78	1.5	54
-	**13**	THF	−78	1.5	5
1	**13**	THF	−78	16	70
-	**13**	THF	−78	16	32
1	**13**	Et_2O	−78	1.5	20
-	**13**	Et_2O	−78	1.5	≤ 1
1	**13**	Et_2O	−78	16	32
-	**13**	Et_2O	−78	16	≤ 1
1	**13**	Toluene	−100	0.16	57
1	**13**	Toluene	−100	0.5	55
1	**13**	Toluene	−100	1.5	58
-	**13**	Toluene	−100	1.5	10
1	**13**	Toluene	−100	7.5	60
-	**13**	Toluene	−100	7.5	10
1	**13**	THF	−100	0.5	51
-	**13**	THF	−100	0.5	≤ 1
1	**13**	THF	−100	1.5	57
1	**13**	THF	−100	3	60
1	**13**	THF	−100	4.5	53
-	**13**	THF	−100	4.5	3

[a] With 20 mol% catalyst loading, for structure see Figure 2 and Scheme S1 and S2. [b] Yield of product **15** and **16** determined by ^{1}H NMR integration.

4.1.2. Catalyst Loading

Vials containing substrate solutions in THF prepared as described in section 4.1. were cooled to −100 °C and 50 – 400 µL of a 0.05 mM stock solution of catalyst **1** in THF were added, corresponding to range of 5 – 40 mol%, 0.0025 – 0.02 mmol, followed by the addition of 600 – 950 µL THF to give a total volume of 1 mL for the added solution. The solutions were stirred for 15 min and subsequently the nucleophile **13** (15 µL, 0.075 mmol) was added and the reaction was stirred for 30 min before quenching by the addition of 0.2 mL of a 0.5 M solution of NaOMe in methanol. The mixture was filtered cold through a silica filled pipette, the product was eluted with EtOAc, the solvent removed in vacuo and the residue was taken up in $CDCl_3$ and analyzed by ^1H NMR spectroscopy. Results are summarized in Table S2.

Table S2: Variation of catalyst loading.

Loading [mol%][a]	η [%][b]
-	≤ 2
5	51
10	61
20	51
30	48
40	49

[a] With catalyst **1**, for structure see Scheme S1 and S2. [b] Yield of product **15** determined by ^1H NMR integration.

4.1.3. Chloride Inhibition

Vials containing substrate solutions in THF prepared as described in section 4.1. were cooled to −100 °C and 338 µL of a 0.029 mM stock solution of catalyst **1** in THF were added, followed by the addition of 33 – 662 µL of a 0.030 mM TBACl stock solution and the addition of 0 – 628 µL THF to give a total volume of 1 mL for the added solution. The solutions were stirred for 20 min and subsequently the nucleophile **13** (15 µL) was added and the reaction was stirred for 30

min before quenching by the addition of 0.2 mL of a 0.5 M solution of NaOMe in methanol. The mixture was filtered cold through a silica filled pipette, the product was eluted with EtOAc, the solvent removed in vacuo and the residue was taken up in $CDCl_3$ and analyzed by ^1H NMR spectroscopy.

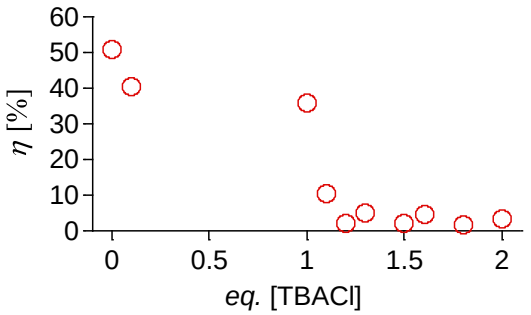


Figure S9. Chloride inhibition study, yield η (%) of product **15** vs increasing equivalents of TBACl relative to catalyst **1**.

4.1.4. Catalyst Screening

Vials containing substrate solutions in THF prepared as described in section 4.1. were cooled to −100 °C and 1 mL stock solution of catalysts **1**-**10** (20 mol%, 0.01 mmol) in THF were added. The solutions were stirred for 20 min and subsequently the nucleophile **13** (15 µL, 0.075 mmol) was added and the reaction was stirred for the appropriate amount of time before quenching by the addition of 0.2 mL of a 0.5 M solution of NaOMe in methanol. The mixture was filtered cold through a silica filled pipette, the product was eluted with EtOAc, the solvent removed in vacuo and the residue was taken up in $CDCl_3$ and analyzed by ^1H NMR spectroscopy.

Table S3: Catalyst screening.

Cat.[a]	E[b]	*t* [h]	η [%][c]
-	-	4.5	≤ 3
1	Sb	4.5	53
8	Sb	4	40
9	Sb	4	3
10	Sb	4	3
2	As	6	3
3	P	6	3
4	Te	5	47
5	Se	5	6
6	I	5	47
7	Br	4	4

[a] With 20 mol% catalyst, for structures see Scheme S1 and S2. [b] Central atom of catalyst, engaged in σ hole interactions. [c] Yield of product **15** determined by ^{1}H NMR integration.

4.1.5. Kinetics

Reactions were run as outlined in section 4.1.4., except for catalyst **1** where the substrate concentration was halved. Reactions were quenched in varying time intervals. The concentration of product **15** was plotted against reaction time, and the initial velocities were determined from linear fitting (Figure S10). Apparent second-order rate constants were determined from Equation (S3).

$$k_{app} = v_{ini} / ([\mathbf{11}]_0\,[\mathbf{15}]_0) \qquad \text{(S3)}$$

ΔE_a was approximated by Equation (S4).

$$k_{cat}/k_{uncat} = \exp\,(-\Delta E_a / RT) \qquad \text{(S4)}$$

Where k_{cat} corresponds to the second-order rate constant of a reaction with catalysts **1**, **4**, **6** and **8** and k_{uncat} to the second-order rate constant of the uncatalyzed reaction.

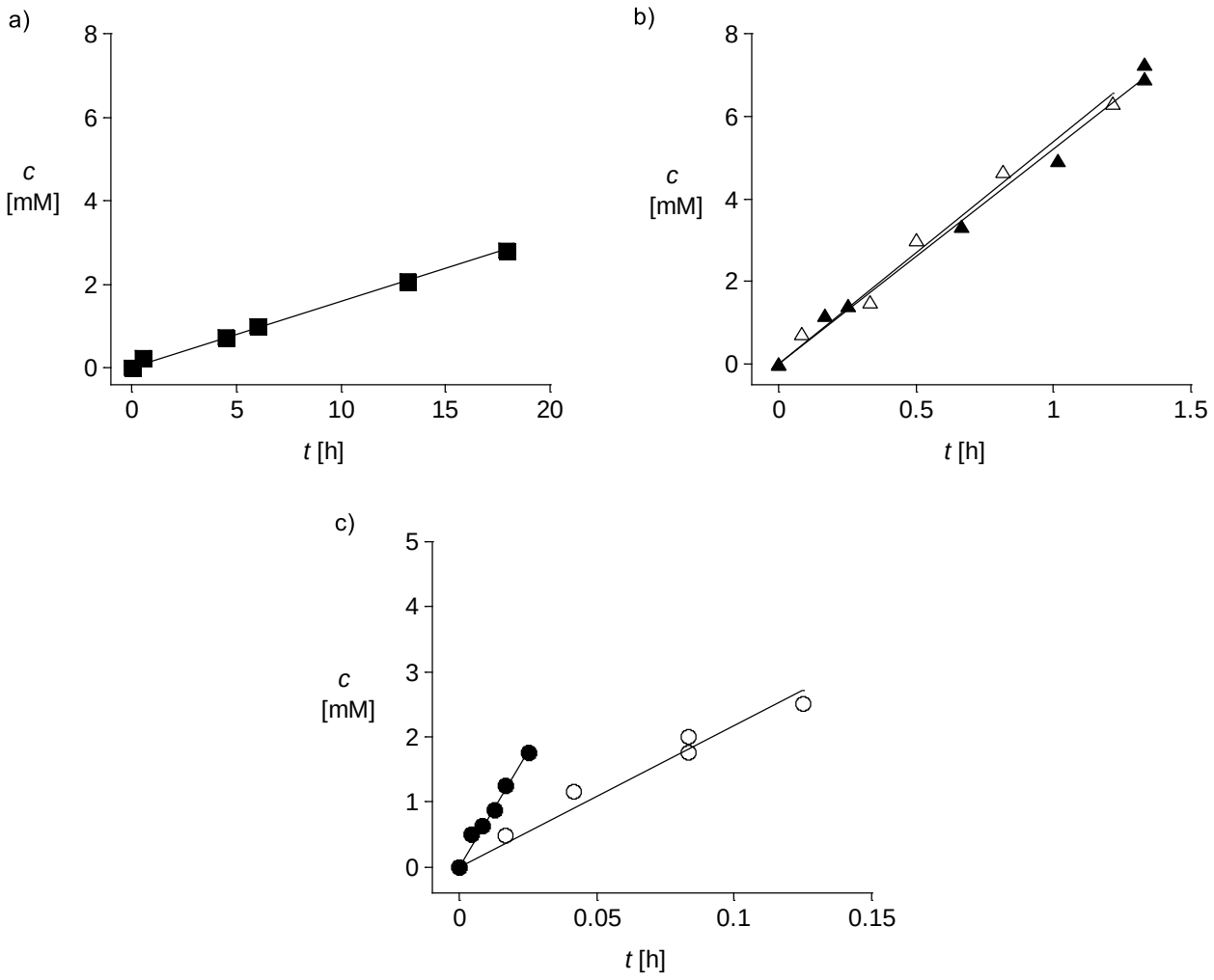


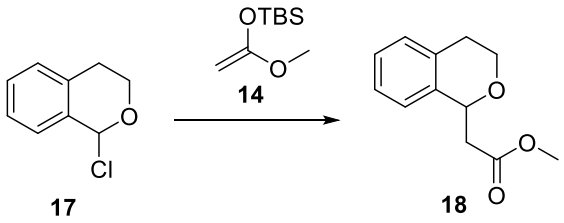
Figure S10. a) Formation of product **15** with time without catalyst, b) with catalyst **4** (△) and **6** (▲), and c) antimony based catalysts **1** (●) and **8** (○).

Table S4: Relative rates and transition-state stabilization.

Cat[a]	k_{app} [mM^{-1} h^{-1}]	k_{cat}/k_{uncat}[b]	ΔE_a [kJ mol^{-1}][c]
-	110	1	-
6	5550	50	9.5
4	5750	52	9.6
1	449860	4090	20.3
8	23040	209	13.0

[a] With 20 mol% catalyst, for structures see Figure 1 and Schemes S1 and S2. [b] Rate enhancement for the formation of product **15** compared to the blank reaction without catalyst with a k_{uncat} = 110 mM^{-1} h^{-1}. [c] Transition-state stabilization calculated from Equation (S4).

4.2. Chloride Abstraction



Scheme S4. Substrate **17** (166.7 mM) was reacted with nucleophile **14** (250 mM) in the presence of catalysts (20 mol%) in dry THF at −78 °C.

As described by Wonner, P. et al in reference [S7] an oven dried microwave vial with a magnetic stir bar freshly taken from the oven was capped with a rubber septum and cooled to rt. A stock solution (0.5 mL) of catalyst (20 mol%, 0.02 mmol) in dry THF was added to the vial and cooled to −78 °C. Successively 1-chloroisochroman (**17**) was added as a 1 M stock solution in dry THF (100 µL, 0.1 mmol) and the mixture was stirred for 20 min before silyl enol ether **14** (15 µL, 0.15 mmol) was added. The reaction mixture was maintained at −78 °C for the desired amount of time until quenching by addition of 0.1 mL of a 5.4 M solution of NaOMe in methanol. The crude reaction mixture was warmed to rt and diluted with chloroform, the solvent was evaporated and the crude residue was dissolved in $CDCl_3$ and analyzed by ^1H NMR spectroscopy. After baseline correction, the product signal of **18** at δ 5.25 ppm was integrated and the signal for 1-methoxyisochroman at δ 5.46 ppm was chosen as a relative standard and the integral was set as 1. Ultimately 100% were divided through the sum of all integrals and multiplied by the respective integral, revealing the appropriate NMR yield for each compound, Figure S11.

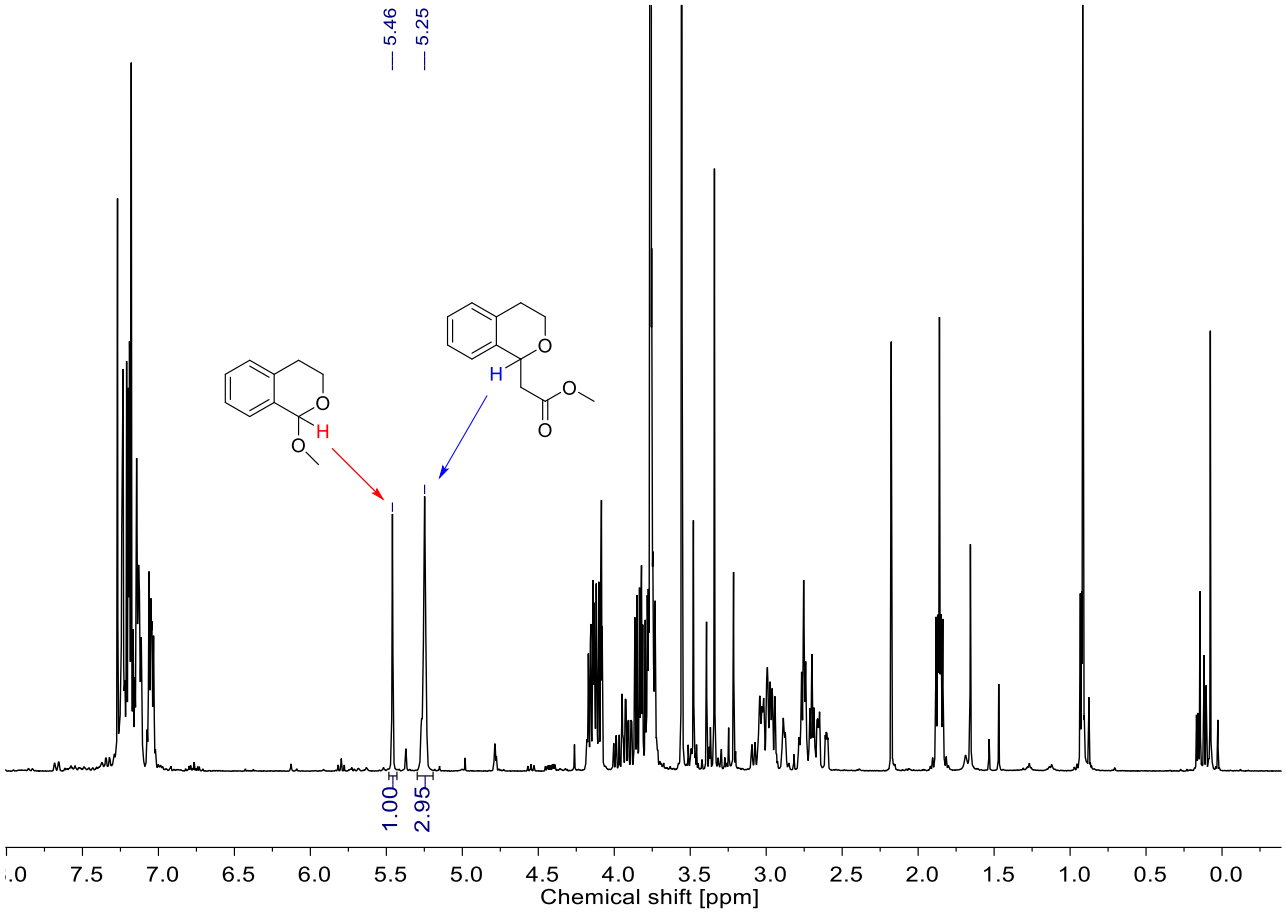


Figure S11. Representative ^{1}H NMR spectra with integrated signals for the unreacted methoxyisochroman (red proton/arrow) at δ 5.46 ppm and product **18** (blue arrow/proton) at δ 5.25 ppm.

4.2.1. Catalyst Screening

The reactions were conducted as described in section 4.2 using stock solutions of catalysts **1, 2** and **4 - 10** (0.5 mL, 20 mol%, 0.05 mmol). After the addition of the nucleophile **14**, the reactions were allowed to react for 55 h at −78 °C before quenching. Results are summarized in Table S5.

Table S5: Catalyst screening.

Cat.[a]	E[b]	η [%][c]
-	-	3[d]
1	Sb	91
8	Sb	30
9	Sb	11
10	Sb	8
2	As	7
3	P	n.d.
4	Te	48
5	Se	6
6	I	15
7	Br	6

[a] With 20 mol% catalyst, for structures see Figure 1 and Scheme S1 and S2. [b] Central atom of catalyst, engaged in σ hole interactions. [c] Yield of product **18** determined by ^{1}H NMR integration after 55 h. [d] Determined after 90 h reaction time.

4.2.2. Kinetics

Reactions were run as outlined in section 4.2 and quenched at varying time intervals. The concentration of product **18** was plotted against reaction time, and the initial velocities were determined from linear fitting (Figure S12). Apparent second-order rate constants were determined from Equation (S5).

$$k_{app} = v_{ini} / ([\mathbf{17}]_0\,[\mathbf{14}]_0) \qquad \text{(S5)}$$

ΔE_a was approximated by Equation (S6).

$$k_{cat}/k_{uncat} = \exp\,(-\Delta E_a / RT) \qquad \text{(S6)}$$

Where k_{cat} corresponds to the second-order rate constant of a reaction with catalysts **1**,**4**, **6** and **8** and k_{uncat} to the second-order rate constant of the uncatalyzed reaction.

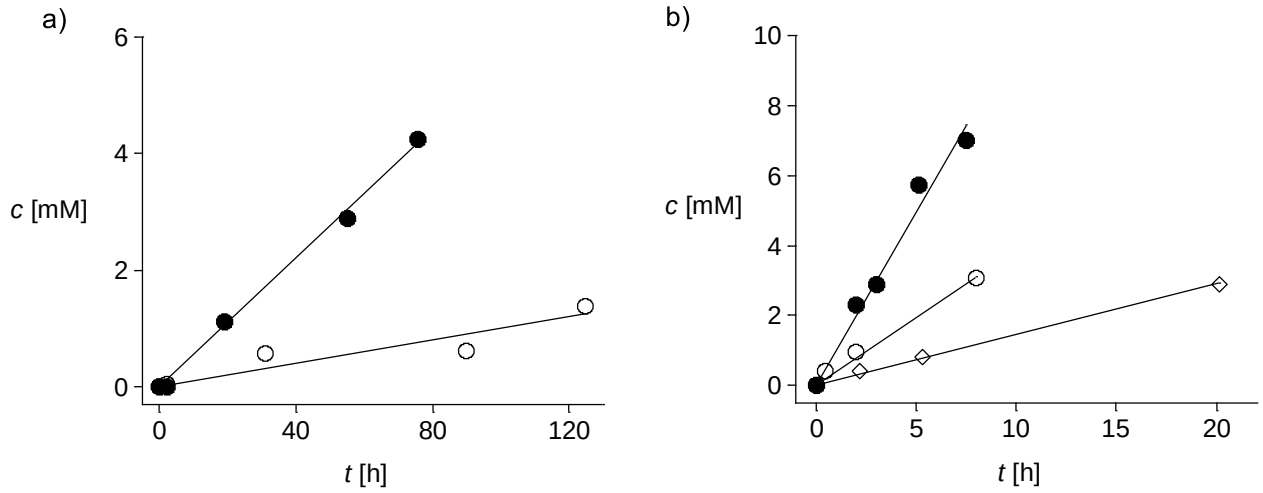


Figure S12. a) Formation of product **14** with time without catalyst (○) and catalyst **6** (●), b) with catalysts **1** (●), **4** (◊) and **8** (○).

Table S6: Relative rates and transition-state stabilization.

Cat[a]	k_{app} [mM^{-1} h^{-1}]	k_{cat}/k_{uncat}[b]	ΔE_a [kJ mol^{-1}][c]
-	168	1	-
6	920	5	4.1
4	6495	39	8.9
1	16590	99	11.2
8	2412	14	6.5

[a] With 20 mol% catalyst, for structures see Figure 2 and scheme S1 and S2. [b] Rate enhancement for formation of product **18** compared to the blank reaction without catalyst with a k_{uncat} = 168 mM^{-1} h^{-1}. [c] Transition-state stabilization calculated from Equation (S6).

5. Computational Studies

Calculations were performed using the Gaussian09 program,[S8] all structures were optimized with and without chloride using M06-2X/6-311G** and the aug_cc-pVTZ-pp basis set for heavy atoms: Br, Se, As, Sb, Te, I. Frequency calculations were performed at the same level to confirm minima (no negative frequencies). Binding energies were compensated for the basis set

superposition error (BSSE) with the counterpoise method.[S9] Structures were visualized with CYLView, molecular electrostatic potential surfaces (MEPs) with Gauss View.

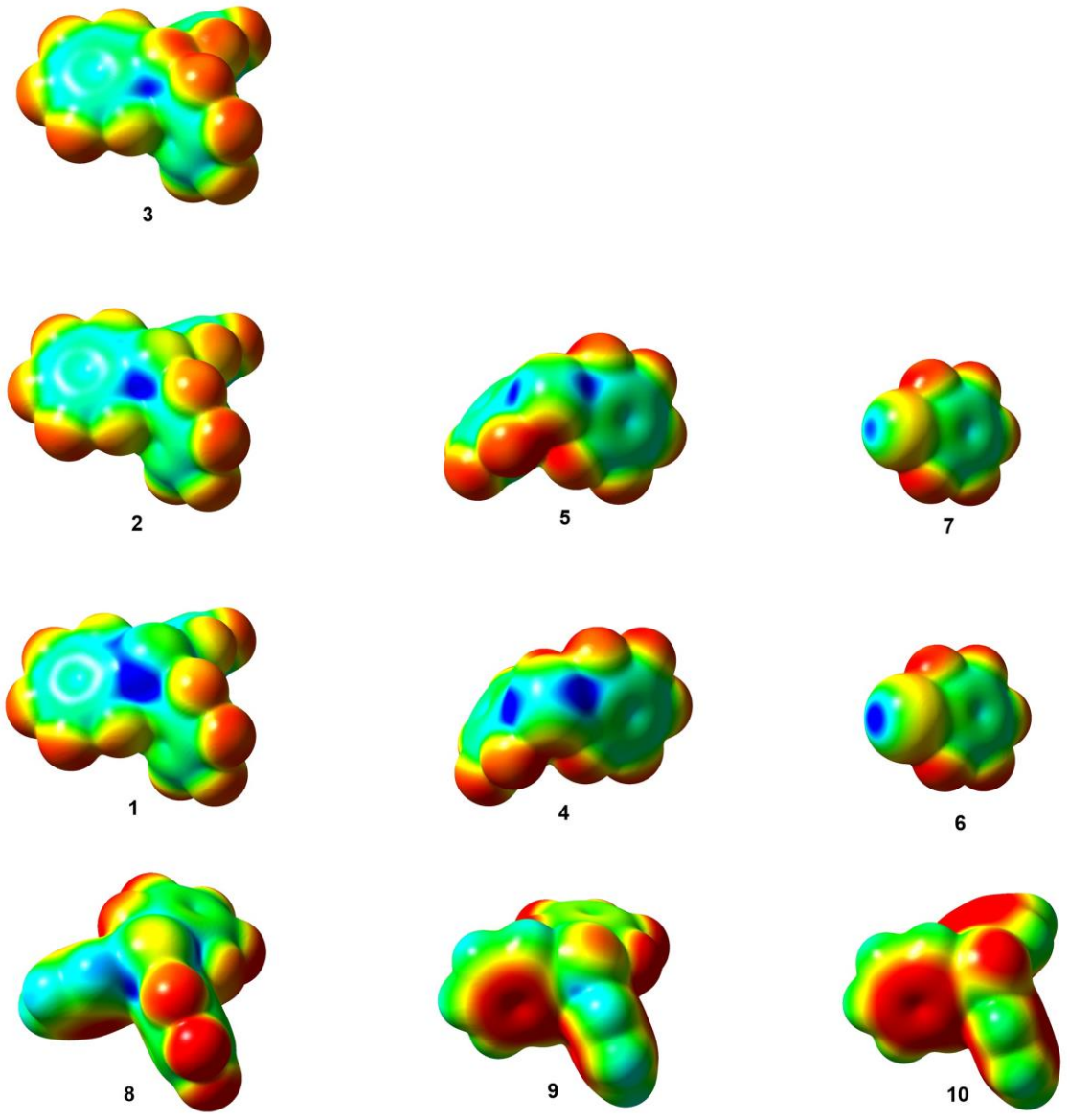


Figure S13. MEP Surfaces of catalysts **1-10**, calculated with M06-2X/6-311G**/aug_cc-pVTZ-pp. Isosurface: 0.001 au; red: -0.01327 au, blue: 0.04527 au.

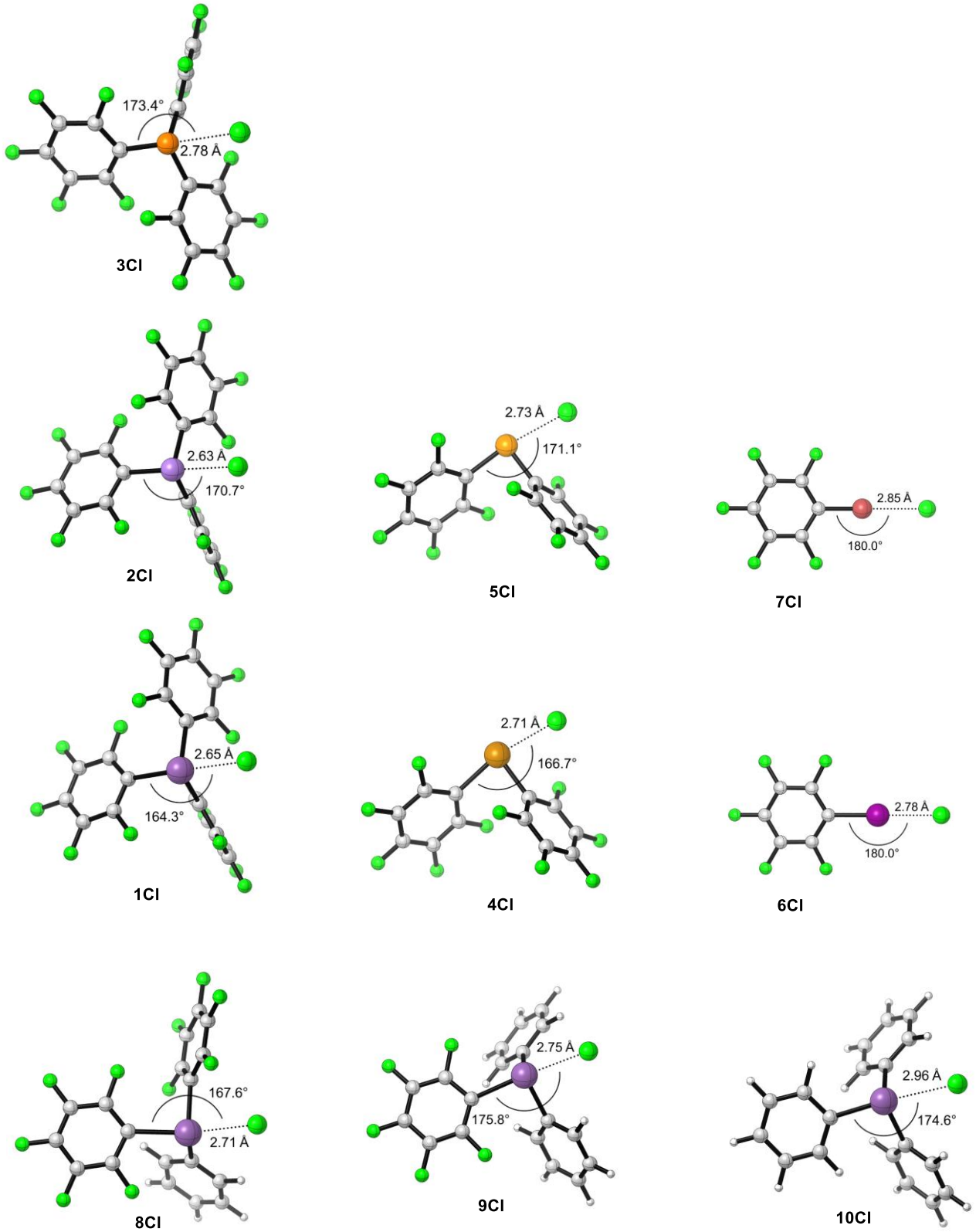


Figure 14. Chloride complexes of catalysts **1**-**10**, calculated with M06-2X/6-311G**/aug_cc-pVTZ-pp.

Table S7: Computational data.

cpd[a]	E_{int} [kcal/mol][b]	d [Å][c]	Θ [°][d]	V_{max}[kcal/mol][e]
1	–51.8	2.64	164.3	–41.1
2	–40.8	2.63	170.6	–32.3
3	–30.0	2.78	173.4	–28.4
4	–39.7	2.71	166.7	–36.7
5	–28.5	2.73	171.1	–29.0
6	–27.8	2.78	180.0	–32.3
7	–17.7	2.84	180.0	–28.6
8	–44.4	2.71	167.5	–28.9
9	–37.2	2.75	175.8	–25.1
10	–22.6	2.95	174.6	n.a.[f]

[a] For structures see Figure 1 and Schemes S1 and S2. [b] Calculated interaction energies for a 1:1 chloride complex. [c] Calculated distance between pnictogen, chalcogen or halogen atom and chloride. [d] Calculated binding angle for chloride. [e] Maximum electrostatic potential at the deepest σ hole, calculated with M06-2X/6-311G**/aug_cc-pVTZ-pp. Isosurface: 0.001 au, for surfaces see Figure S13. [f] No clear σ hole could be identified.

6. Supporting References

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7. Computational Data

Tris(pentafluorophenyl)stibine 1

Zero-point correction = 0.151592 (Hartree/Particle)

Thermal correction to Energy = 0.181798

Thermal correction to Enthalpy = 0.182742

Thermal correction to Gibbs Free Energy = 0.087693

Sum of electronic and zero-point Energies = -2423.308882

Sum of electronic and Thermal Energies = -2423.278676

Sum of electronic and Thermal Enthalpies = -2423.277732

Sum of electronic and Thermal Free Energies = -2423.372781

C	0.636969	-1.286686	2.397080
C	-0.047111	-0.153119	1.988463
C	-0.489826	0.713380	2.971195
C	-0.270622	0.474508	4.319090
C	0.414102	-0.670369	4.693816
C	0.873866	-1.560288	3.731895
Sb	-0.386204	0.324399	-0.090311
C	1.725430	0.079847	-0.544203
C	2.384673	-1.014838	-1.079257
C	3.749490	-0.997811	-1.326257
C	4.487012	0.136416	-1.025044
C	3.861980	1.245870	-0.476163
C	2.498469	1.191523	-0.250181
C	-1.053794	-1.634838	-0.727951
C	-1.672917	-2.593124	0.053377

C	-2.134676	-3.786007	-0.482134
C	-1.983646	-4.026775	-1.839054
C	-1.377299	-3.080432	-2.653274
C	-0.934616	-1.904238	-2.079613
F	-1.851980	-2.394636	1.363539
F	-0.337291	-0.993659	-2.864741
F	-1.232207	-3.313831	-3.950686
F	-2.423383	-5.161138	-2.359679
F	-2.723505	-4.693522	0.286272
F	-1.153165	1.824152	2.632445
F	-0.705317	1.319393	5.244593
F	0.631969	-0.917854	5.975113
F	1.523535	-2.654862	4.104999
F	1.075611	-2.162349	1.488298
F	1.734884	-2.141907	-1.365954
F	4.357137	-2.059418	-1.839321
F	5.790077	0.158486	-1.254001
F	4.567861	2.327705	-0.175580
F	1.906762	2.267031	0.295327

Tris(pentafluorophenyl)stibine complex with Cl^-, 1Cl

Zero-point correction = 0.151412 (Hartree/Particle)

Thermal correction to Energy = 0.183773

Thermal correction to Enthalpy = 0.184717

Thermal correction to Gibbs Free Energy = 0.085049

Sum of electronic and zero-point Energies = -2883.647860

Sum of electronic and Thermal Energies = -2883.615499

Sum of electronic and Thermal Enthalpies = -2883.614555

Sum of electronic and Thermal Free Energies = -2883.714223

C	-0.431005	-2.173104	-1.895039
C	-1.101061	-1.526529	-0.871197
C	-2.232454	-2.147305	-0.379579
C	-2.697932	-3.359424	-0.856129
C	-2.001010	-3.982811	-1.876973
C	-0.862849	-3.391183	-2.398165
Sb	-0.645380	0.450658	-0.078705
C	1.507173	0.493437	-0.412486
C	2.341682	-0.607161	-0.329306
C	3.708602	-0.516681	-0.539259
C	4.268915	0.716719	-0.825762
C	3.466232	1.842442	-0.895936
C	2.102819	1.711989	-0.684387
F	1.852632	-1.818079	-0.040053
F	4.491377	-1.595022	-0.466161
F	5.583144	0.821876	-1.022539
F	4.017567	3.030248	-1.151322
F	1.365207	2.824367	-0.727274
F	-2.914836	-1.575186	0.627648
F	-3.791706	-3.932960	-0.349372
F	-2.424149	-5.153261	-2.354507
F	-0.197664	-4.004012	-3.379313
F	0.672233	-1.658240	-2.434122

C 0.013584 -0.543108 1.961573

C -0.059190 -1.837992 2.438410

C 0.347357 -2.202022 3.715220

C 0.858445 -1.237665 4.566599

C 0.958485 0.073324 4.133160

C 0.534758 0.378062 2.849785

F -0.522469 -2.840499 1.670721

F 0.664549 1.669224 2.465148

F 1.459303 1.005083 4.950894

F 1.256143 -1.571130 5.796853

F 0.263425 -3.467924 4.137316

Cl -0.819746 1.184850 -2.615246

Tris(pentafluorophenyl)arsine 2

Zero-point correction = 0.152853 (Hartree/Particle)

Thermal correction to Energy = 0.182486

Thermal correction to Enthalpy = 0.183431

Thermal correction to Gibbs Free Energy = 0.090824

Sum of electronic and zero-point Energies = -2515.760320

Sum of electronic and Thermal Energies = -2515.730687

Sum of electronic and Thermal Enthalpies = -2515.729743

Sum of electronic and Thermal Free Energies = -2515.822350

C 0.714295 -1.359328 2.382883

C 0.019541 -0.258265 1.903352

C -0.471904 0.645730 2.830429

C -0.288726 0.467680 4.193611

C 0.404185 -0.644346 4.641629

C	0.911163	-1.566387	3.735011
As	-0.252043	0.116788	-0.005707
C	1.667728	-0.032836	-0.462897
C	2.366613	-1.099710	-1.009118
C	3.716350	-1.004492	-1.315302
C	4.399667	0.174299	-1.065261
C	3.733901	1.254044	-0.506346
C	2.386830	1.129565	-0.218488
C	-0.911568	-1.629671	-0.629767
C	-1.584357	-2.578319	0.122469
C	-2.125029	-3.717158	-0.456660
C	-2.006765	-3.914662	-1.822511
C	-1.353159	-2.973986	-2.605562
C	-0.830256	-1.850527	-1.996383
F	-1.746793	-2.429449	1.439065
F	-0.194210	-0.951126	-2.756629
F	-1.239123	-3.160111	-3.913176
F	-2.521874	-4.997455	-2.381435
F	-2.759523	-4.613879	0.286882
F	-1.142016	1.725211	2.428080
F	-0.769161	1.345211	5.063978
F	0.583543	-0.831905	5.938391
F	1.566364	-2.632083	4.175682
F	1.192158	-2.267662	1.532314
F	1.779901	-2.268459	-1.254619
F	4.359254	-2.040168	-1.837931

F 5.687838 0.266068 -1.352064

F 4.385638 2.381200 -0.255177

F 1.763809 2.177198 0.333354

Tris(pentafluorophenyl)arsine complex with Cl^-, 2Cl

Zero-point correction = 0.152649 (Hartree/Particle)

Thermal correction to Energy = 0.184457

Thermal correction to Enthalpy = 0.185401

Thermal correction to Gibbs Free Energy = 0.087887

Sum of electronic and zero-point Energies = -2976.083414

Sum of electronic and Thermal Energies = -2976.051605

Sum of electronic and Thermal Enthalpies = -2976.050661

Sum of electronic and Thermal Free Energies = -2976.148176

C -0.337883 -2.171326 -1.832672

C -0.942725 -1.539130 -0.757588

C -2.092999 -2.121324 -0.257088

C -2.634976 -3.284639 -0.772944

C -2.004235 -3.897225 -1.840731

C -0.852515 -3.340913 -2.369965

As -0.480302 0.224473 0.009561

C 1.456291 0.351448 -0.380055

C 2.347095 -0.708469 -0.333254

C 3.697045 -0.549686 -0.596526

C 4.186773 0.712049 -0.887924

C 3.329252 1.798032 -0.904765

C 1.980711 1.607374 -0.645021

F 1.931947 -1.941194 -0.027289

F	4.530351	-1.591442	-0.561985
F	5.485366	0.881912	-1.133765
F	3.814822	3.015067	-1.153589
F	1.204832	2.685535	-0.626489
F	-2.711607	-1.562890	0.794375
F	-3.740553	-3.821669	-0.252905
F	-2.500076	-5.023067	-2.354203
F	-0.247652	-3.942596	-3.395645
F	0.770292	-1.697172	-2.391417
C	0.097601	-0.605119	1.893487
C	0.058716	-1.892101	2.400876
C	0.407096	-2.196203	3.710458
C	0.824783	-1.187137	4.559937
C	0.891155	0.114106	4.092408
C	0.528527	0.367567	2.780295
F	-0.305888	-2.938253	1.644115
F	0.624586	1.645387	2.363503
F	1.302707	1.091010	4.905262
F	1.165444	-1.466645	5.819265
F	0.355972	-3.452314	4.163109
Cl	-0.851556	1.035945	-2.467364

Tris(pentafluorophenyl)phosphine 3

Zero-point correction = 0.151592 (Hartree/Particle)

Thermal correction to Energy = 0.181798

Thermal correction to Enthalpy = 0.182742

Thermal correction to Gibbs Free Energy = 0.087693

Sum of electronic and zero-point Energies = -2423.308882

Sum of electronic and Thermal Energies = -2423.278676

Sum of electronic and Thermal Enthalpies = -2423.277732

Sum of electronic and Thermal Free Energies = -2423.372781

C	0.751901	-1.399128	2.377563
C	0.043982	-0.323656	1.851012
C	-0.464909	0.609338	2.744263
C	-0.283116	0.480186	4.113989
C	0.422480	-0.604102	4.605499
C	0.943891	-1.554120	3.735941
P	-0.176097	-0.022689	0.047073
C	1.621607	-0.102899	-0.408548
C	2.349806	-1.155584	-0.952017
C	3.688557	-1.018727	-1.287641
C	4.338961	0.183313	-1.064725
C	3.647651	1.247687	-0.508592
C	2.310601	1.087976	-0.193025
C	-0.831775	-1.630077	-0.579618
C	-1.528333	-2.584550	0.149489
C	-2.110446	-3.687042	-0.459718
C	-2.019439	-3.846062	-1.831514
C	-1.343165	-2.902927	-2.590986
C	-0.777857	-1.814653	-1.957408
F	-1.672108	-2.483327	1.471100
F	-0.123866	-0.919401	-2.701790
F	-1.248865	-3.049516	-3.904891

F -2.575415 -4.893979 -2.416547

F -2.761046 -4.585355 0.267318

F -1.144584 1.663577 2.307993

F -0.777961 1.383357 4.948598

F 0.599655 -0.741502 5.908146

F 1.611134 -2.593062 4.218901

F 1.242662 -2.329381 1.561621

F 1.799668 -2.344964 -1.175929

F 4.352700 -2.040977 -1.809326

F 5.617985 0.311661 -1.375840

F 4.266270 2.398303 -0.283027

F 1.671739 2.123289 0.354734

Tris(pentafluorophenyl)phosphine complex with Cl^-, 3Cl

Zero-point correction = 0.154697 (Hartree/Particle)

Thermal correction to Energy = 0.185744

Thermal correction to Enthalpy = 0.186688

Thermal correction to Gibbs Free Energy = 0.091735

Sum of electronic and zero-point Energies = -2984.771234

Sum of electronic and Thermal Energies = -2984.740187

Sum of electronic and Thermal Enthalpies = -2984.739242

Sum of electronic and Thermal Free Energies = -2984.834195

C -0.802423 -1.782655 -2.030946

C -0.852327 -1.636141 -0.652747

C -1.449275 -2.668436 0.060644

C -1.963398 -3.786415 -0.576255

C -1.900161 -3.894316 -1.954163

C	-1.311275	-2.884340	-2.692238
P	-0.315101	0.020444	-0.021061
C	1.581410	-0.168007	-0.388400
C	2.312434	-1.195643	-0.969254
C	3.664552	-1.077089	-1.263396
C	4.338117	0.090945	-0.958521
C	3.652923	1.133468	-0.358776
C	2.304474	0.982899	-0.089092
F	1.760995	-2.373997	-1.272924
F	4.327562	-2.088272	-1.827450
F	5.636257	0.211056	-1.233540
F	4.296116	2.260499	-0.050661
F	1.686695	2.012840	0.503983
F	-1.547501	-2.647107	1.382620
F	-2.523162	-4.768312	0.131044
F	-2.394594	-4.969969	-2.565909
F	-1.230185	-2.985650	-4.020275
F	-0.210863	-0.836107	-2.772258
C	-0.011993	-0.236969	1.787745
C	0.629316	-1.342795	2.328328
C	0.847356	-1.480512	3.687237
C	0.453753	-0.463689	4.540298
C	-0.142322	0.675166	4.028929
C	-0.358756	0.786213	2.663681
F	1.055661	-2.332774	1.539583
F	-0.874109	1.920657	2.222068

F -0.480986 1.664837 4.854710

F 0.666701 -0.575591 5.850104

F 1.442391 -2.568232 4.180796

Cl -2.986763 0.072029 0.735712

Bis(pentafluorophenyl)tellane 4

Zero-point correction = 0.101077 (Hartree/Particle)

Thermal correction to Energy = 0.121338

Thermal correction to Enthalpy = 0.122282

Thermal correction to Gibbs Free Energy = 0.049181

Sum of electronic and zero-point Energies = -1723.351022

Sum of electronic and Thermal Energies = -1723.330761

Sum of electronic and Thermal Enthalpies = -1723.329817

Sum of electronic and Thermal Free Energies = -1723.402919

C 0.209729 -1.625559 -1.952696

C 0.652674 -0.766951 -0.957330

C 2.000842 -0.795174 -0.626572

C 2.884000 -1.657914 -1.253957

C 2.416041 -2.505265 -2.246898

C 1.076261 -2.490656 -2.602106

Te -0.681945 0.513147 0.064141

C -0.163142 -0.327531 1.931599

C -0.294930 -1.691333 2.156152

C 0.080324 -2.268457 3.357829

C 0.587025 -1.465168 4.368221

C 0.720617 -0.099390 4.172751

C 0.347771 0.453577 2.957757

F -0.778518 -2.490317 1.206957

F 0.496324 1.765897 2.798108

F 1.208182 0.661912 5.143424

F 0.943312 -2.003943 5.523169

F -0.046579 -3.574361 3.554024

F 2.482338 0.005964 0.321879

F 4.168249 -1.676473 -0.921773

F 3.251298 -3.329840 -2.858072

F 0.635978 -3.305812 -3.551414

F -1.071547 -1.641549 -2.310225

Bis(pentafluorophenyl)tellane complex with Cl^-, 4Cl

Zero-point correction = 0.100819 (Hartree/Particle)

Thermal correction to Energy = 0.123376

Thermal correction to Enthalpy = 0.124320

Thermal correction to Gibbs Free Energy = 0.045460

Sum of electronic and zero-point Energies = -2183.674955

Sum of electronic and Thermal Energies = -2183.652399

Sum of electronic and Thermal Enthalpies = -2183.651455

Sum of electronic and Thermal Free Energies = -2183.730314

C 0.407606 0.499142 2.760898

C -0.235464 -0.272478 1.803442

C -0.452387 -1.608082 2.099649

C -0.059144 -2.166006 3.306998

C 0.567886 -1.371046 4.248957

C 0.804039 -0.033851 3.976590

Te -0.890479 0.567786 -0.027671

C	0.629512	-0.800601	-0.968690
C	0.284830	-1.622487	-2.026729
C	1.186151	-2.477759	-2.643645
C	2.493063	-2.522224	-2.189916
C	2.881075	-1.711773	-1.136067
C	1.949110	-0.865601	-0.554235
F	-0.966849	-1.623051	-2.510286
F	2.390117	-0.091869	0.449320
F	4.147473	-1.752231	-0.709069
F	3.377374	-3.337627	-2.769632
F	0.817190	-3.260302	-3.663279
F	-1.052772	-2.418512	1.225346
F	-0.282479	-3.456166	3.572966
F	0.952198	-1.893242	5.414652
F	1.428688	0.718417	4.885445
F	0.690004	1.775579	2.536904
Cl	-2.544190	1.928396	1.636829

Bis(pentafluorophenyl)selane 5

Zero-point correction = 0.101930 (Hartree/Particle)

Thermal correction to Energy = 0.121874

Thermal correction to Enthalpy = 0.122818

Thermal correction to Gibbs Free Energy = 0.051010

Sum of electronic and zero-point Energies = -1828.758953

Sum of electronic and Thermal Energies = -1828.739009

Sum of electronic and Thermal Enthalpies = -1828.738064

Sum of electronic and Thermal Free Energies = -1828.809873

C	0.191911	-1.647146	-1.813230
C	0.655212	-0.770417	-0.841591
C	2.019320	-0.738407	-0.578819
C	2.901703	-1.565755	-1.252073
C	2.418129	-2.432105	-2.221409
C	1.062607	-2.473210	-2.507284
Se	-0.552978	0.356312	0.125927
C	-0.120351	-0.382102	1.838501
C	-0.333840	-1.729466	2.103169
C	-0.004108	-2.283728	3.328102
C	0.534719	-1.475468	4.318202
C	0.747013	-0.126842	4.079505
C	0.423192	0.408241	2.842115
F	-0.849423	-2.524720	1.171710
F	0.652636	1.699103	2.637435
F	1.267755	0.637958	5.029434
F	0.848159	-1.994376	5.494261
F	-0.204732	-3.573308	3.565095
F	2.507757	0.083565	0.344161
F	4.200581	-1.532521	-0.985395
F	3.253985	-3.223073	-2.874369
F	0.607452	-3.308085	-3.431549
F	-1.102395	-1.719645	-2.096930

Bis(pentafluorophenyl)selane complex with Cl^-, 5Cl

Zero-point correction = 0.101200 (Hartree/Particle)

Thermal correction to Energy = 0.122699

Thermal correction to Enthalpy = 0.123643

Thermal correction to Gibbs Free Energy = 0.048655

Sum of electronic and zero-point Energies = -2289.068382

Sum of electronic and Thermal Energies = -2289.046883

Sum of electronic and Thermal Enthalpies = -2289.045938

Sum of electronic and Thermal Free Energies = -2289.120927

C	0.382708	0.378724	2.957205
C	-0.085328	-0.369800	1.888841
C	-0.248376	-1.729992	2.106212
C	0.054211	-2.330458	3.318012
C	0.522402	-1.552341	4.363802
C	0.685399	-0.189722	4.186058
Se	-0.549602	0.517861	0.151205
C	0.606455	-0.691737	-0.776202
C	0.093763	-1.637367	-1.655480
C	0.931345	-2.461014	-2.387939
C	2.304659	-2.356720	-2.238421
C	2.835501	-1.434514	-1.355243
C	1.982306	-0.613044	-0.634348
F	-1.210331	-1.790957	-1.809104
F	2.535340	0.261751	0.205584
F	4.160256	-1.342216	-1.209523
F	3.113304	-3.153502	-2.938739
F	0.432395	-3.368279	-3.229946
F	-0.712409	-2.524168	1.135951
F	-0.110811	-3.643479	3.499322

F 0.810841 -2.114266 5.538945

F 1.138655 0.556437 5.196991

F 0.564471 1.696968 2.840095

Cl -0.876604 1.485450 -2.385204

Iodopentafluorobenzene 6

Zero-point correction = 0.050523 (Hartree/Particle)

Thermal correction to Energy = 0.060757

Thermal correction to Enthalpy = 0.061701

Thermal correction to Gibbs Free Energy = 0.012917

Sum of electronic and zero-point Energies = -1023.322500

Sum of electronic and Thermal Energies = -1023.312267

Sum of electronic and Thermal Enthalpies = -1023.311323

Sum of electronic and Thermal Free Energies = -1023.360107

C 0.499688 -2.155122 3.629027

C 0.272045 -1.712735 2.335045

C -0.012685 -0.380290 2.077790

C -0.066419 0.509033 3.142018

C 0.159179 0.079551 4.439694

C 0.442589 -1.255887 4.681675

F 0.333426 -2.597447 1.347838

I -0.353482 0.273331 0.138781

F -0.335526 1.792547 2.940397

F 0.105578 0.937252 5.450070

F 0.658838 -1.671604 5.919832

F 0.771248 -3.431853 3.863943

Iodopentafluorobenzene complex with Cl^-, 6Cl

Zero-point correction = 0.050446 (Hartree/Particle)

Thermal correction to Energy = 0.063007

Thermal correction to Enthalpy = 0.063951

Thermal correction to Gibbs Free Energy = 0.008839

Sum of electronic and zero-point Energies = -1483.630377

Sum of electronic and Thermal Energies = -1483.617816

Sum of electronic and Thermal Enthalpies = -1483.616872

Sum of electronic and Thermal Free Energies = -1483.671985

C	0.490770	-1.454357	4.762802
C	0.495236	-2.160083	3.572012
C	0.235484	-1.495203	2.382781
C	-0.031909	-0.136620	2.334675
C	-0.028640	0.539586	3.543945
C	0.227246	-0.095516	4.750162
F	0.750150	-3.472799	3.587451
F	0.253739	-2.230053	1.266136
I	-0.436426	0.883240	0.455906
F	-0.276175	1.852345	3.595764
F	0.223608	0.583601	5.902217
F	0.739089	-2.080470	5.916425
Cl	-0.954146	2.188306	-1.948098

Bromopentafluorobenzene 7

Zero-point correction = 0.050976 (Hartree/Particle)

Thermal correction to Energy = 0.061040

Thermal correction to Enthalpy = 0.061984

Thermal correction to Gibbs Free Energy = 0.014214

Sum of electronic and zero-point Energies = -1144.728358

Sum of electronic and Thermal Energies = -1144.718294

Sum of electronic and Thermal Enthalpies = -1144.717349

Sum of electronic and Thermal Free Energies = -1144.765120

C 0.497075 -2.149857 3.612865

C 0.269021 -1.709551 2.318333

C -0.015800 -0.375506 2.065295

C -0.070028 0.516749 3.127838

C 0.156836 0.084445 4.424196

C 0.440815 -1.250974 4.665784

F 0.328371 -2.588394 1.327912

Br -0.322049 0.213454 0.318696

F -0.339518 1.797850 2.921169

F 0.103405 0.942089 5.434286

F 0.657687 -1.666771 5.903984

F 0.768665 -3.426754 3.845753

Bromopentafluorobenzene complex with Cl^-, 7Cl

Zero-point correction = 0.050945 (Hartree/Particle)

Thermal correction to Energy = 0.063403

Thermal correction to Enthalpy = 0.064347

Thermal correction to Gibbs Free Energy = 0.009709

Sum of electronic and zero-point Energies = -1605.022866

Sum of electronic and Thermal Energies = -1605.010408

Sum of electronic and Thermal Enthalpies = -1605.009464

Sum of electronic and Thermal Free Energies = -1605.064102

C 0.484813 -1.426254 4.761062

C 0.493855 -2.152516 3.582596

C 0.239481 -1.514447 2.378169

C -0.030716 -0.154482 2.313816

C -0.035269 0.550289 3.510477

C 0.219675 -0.068030 4.724200

F 0.749956 -3.462654 3.618722

F 0.259302 -2.258750 1.273976

Br -0.382276 0.715746 0.650260

F -0.283867 1.858644 3.528951

F 0.210791 0.632079 5.861473

F 0.730102 -2.031690 5.925015

Cl -0.905945 2.012003 -1.827706

Bis(pentafluorophenyl)(phenyl)stibine 8

Zero-point correction = 0.191609 (Hartree/Particle)

Thermal correction to Energy = 0.217411

Thermal correction to Enthalpy = 0.218355

Thermal correction to Gibbs Free Energy = 0.132250

Sum of electronic and zero-point Energies = -1927.108911

Sum of electronic and Thermal Energies = -1927.083109

Sum of electronic and Thermal Enthalpies = -1927.082165

Sum of electronic and Thermal Free Energies = -1927.168270

C 0.261670 -1.696135 2.383527

C -0.032843 -0.362132 2.093650

C -0.085271 0.567285 3.133815

C 0.163349 0.174128 4.446160

C 0.457677 -1.154079 4.725614

C	0.504925	-2.087891	3.694572
Sb	-0.398496	0.387222	0.117353
C	1.692526	0.313057	-0.480014
C	2.466709	-0.834748	-0.527741
C	3.804848	-0.811801	-0.879747
C	4.402725	0.402079	-1.186963
C	3.662773	1.572051	-1.142979
C	2.323487	1.504720	-0.791500
C	-1.000857	-1.514712	-0.743377
C	-2.018308	-2.220430	-0.123084
C	-2.491745	-3.429124	-0.606411
C	-1.942706	-3.946013	-1.769519
C	-0.941182	-3.253315	-2.433455
C	-0.494150	-2.049064	-1.915266
F	-2.580611	-1.727660	0.987986
F	0.461191	-1.401908	-2.592760
F	-0.428843	-3.747332	-3.553724
F	-2.380145	-5.099119	-2.252599
F	-3.459434	-4.087581	0.019818
H	-0.324529	1.607237	2.930320
H	0.120749	0.903542	5.246237
H	0.646701	-1.464839	5.746270
H	0.731643	-3.124911	3.912784
H	0.309944	-2.432908	1.589331
F	1.927893	-2.025377	-0.240156
F	4.522114	-1.928093	-0.925216

F 5.684223 0.441476 -1.519523

F 4.239721 2.732903 -1.429793

F 1.636525 2.654480 -0.751511

Bis(pentafluorophenyl)(phenyl)stibine complex with Cl^-, 8Cl

Zero-point correction = 0.191710 (Hartree/Particle)

Thermal correction to Energy = 0.219616

Thermal correction to Enthalpy = 0.220560

Thermal correction to Gibbs Free Energy = 0.130236

Sum of electronic and zero-point Energies = -2387.434410

Sum of electronic and Thermal Energies = -2387.406505

Sum of electronic and Thermal Enthalpies = -2387.405560

Sum of electronic and Thermal Free Energies = -2387.495884

C -0.148888 -2.159724 -1.601170

C -0.759912 -1.430413 -0.599191

C -1.973867 -1.937206 -0.168955

C -2.554458 -3.093985 -0.661413

C -1.894816 -3.795683 -1.657174

C -0.684307 -3.326087 -2.134005

Sb -0.223668 0.661808 0.335996

C 1.777117 0.499202 -0.533583

C 2.726487 -0.452269 -0.216551

C 4.002848 -0.441165 -0.755730

C 4.346511 0.548178 -1.660261

C 3.414501 1.506068 -2.019823

C 2.151016 1.462244 -1.454069

F 2.434186 -1.457965 0.616747

F	4.901572	-1.374145	-0.427484
F	5.569073	0.571090	-2.194284
F	3.744607	2.446727	-2.908874
F	1.275461	2.392705	-1.850659
F	-2.659083	-1.288004	0.795211
F	-3.727320	-3.544487	-0.203838
F	-2.427965	-4.913412	-2.157751
F	-0.053507	-4.003327	-3.099941
F	1.026380	-1.772293	-2.131673
C	0.008935	-0.345892	2.253402
C	0.154547	-1.728791	2.393288
C	0.153233	-2.326876	3.649151
C	-0.006627	-1.553099	4.793206
C	-0.158449	-0.177959	4.669473
C	-0.148782	0.420144	3.411803
H	-0.243801	1.496908	3.334868
H	-0.279921	0.438845	5.553303
H	-0.009390	-2.018659	5.772804
H	0.280374	-3.400959	3.730293
H	0.289901	-2.352961	1.518701
Cl	0.935701	2.845414	1.441428

(Pentafluorophenyl)bis(phenyl)stibine 9

Zero-point correction = 0.232273 (Hartree/Particle)

Thermal correction to Energy = 0.253663

Thermal correction to Enthalpy = 0.254607

Thermal correction to Gibbs Free Energy = 0.177941

Sum of electronic and zero-point Energies = -1430.904264

Sum of electronic and Thermal Energies = -1430.882874

Sum of electronic and Thermal Enthalpies = -1430.881930

Sum of electronic and Thermal Free Energies = -1430.958596

C	-1.624400	-2.434253	0.063185
C	-0.987094	-1.452421	-0.677538
C	-0.868808	-1.682461	-2.039295
C	-1.326493	-2.836314	-2.651784
C	-1.945100	-3.804305	-1.875038
C	-2.097495	-3.604901	-0.512765
Sb	-0.249245	0.454352	0.084908
C	1.781611	0.117771	-0.531103
C	2.294850	-1.128811	-0.895698
C	3.633641	-1.265751	-1.248441
C	4.476266	-0.158835	-1.237561
C	3.976871	1.086498	-0.875425
C	2.636100	1.222615	-0.528838
C	0.030544	-0.128836	2.134394
C	-0.905294	0.309850	3.073442
C	-0.778782	-0.035953	4.414954
C	0.292344	-0.818525	4.830310
C	1.236628	-1.249439	3.904379
C	1.108514	-0.905176	2.562202
H	-1.746840	0.922135	2.762493
H	-1.514475	0.306527	5.133141
H	0.393717	-1.088794	5.874892

H	2.075837	-1.854651	4.226926
H	1.857451	-1.241219	1.852595
H	1.654400	-2.005278	-0.900966
H	4.019157	-2.238130	-1.532197
H	5.518339	-0.267246	-1.513674
H	4.627617	1.953090	-0.867348
H	2.259542	2.204820	-0.257474
F	-0.283839	-0.757502	-2.813367
F	-1.187752	-3.024991	-3.959454
F	-2.397297	-4.916495	-2.437743
F	-2.697792	-4.532321	0.225536
F	-1.820452	-2.284043	1.374449

(Pentafluorophenyl)bis(phenyl)stibine complex with Cl^-, 9Cl

Zero-point correction = 0.231942 (Hartree/Particle)

Thermal correction to Energy = 0.255397

Thermal correction to Enthalpy = 0.256341

Thermal correction to Gibbs Free Energy = 0.175936

Sum of electronic and zero-point Energies = -1891.220865

Sum of electronic and Thermal Energies = -1891.197410

Sum of electronic and Thermal Enthalpies = -1891.196466

Sum of electronic and Thermal Free Energies = -1891.276871

C	0.595548	-1.300593	2.426122
C	-0.099404	-0.123863	2.144881
C	-0.661668	0.584853	3.207158
C	-0.542425	0.122800	4.515262
C	0.152008	-1.051591	4.781560

C	0.726303	-1.761256	3.732432
Sb	-0.365165	0.618360	0.123465
C	1.708626	0.326665	-0.495383
C	2.257562	-0.942208	-0.706527
C	3.576657	-1.101706	-1.119543
C	4.377022	0.012187	-1.342921
C	3.845711	1.280891	-1.144948
C	2.527284	1.437129	-0.722939
C	-0.872312	-1.567387	-0.617425
C	-1.608868	-2.511877	0.074336
C	-2.040342	-3.707510	-0.486391
C	-1.753671	-3.974439	-1.813482
C	-1.051579	-3.043308	-2.560566
C	-0.643480	-1.868376	-1.948591
F	-1.969153	-2.307453	1.353599
F	0.011375	-0.988009	-2.731409
F	-0.793729	-3.293881	-3.849931
F	-2.165077	-5.115642	-2.375292
F	-2.737424	-4.602220	0.225527
H	-1.170746	1.522899	3.013886
H	-0.984976	0.688933	5.327747
H	0.249862	-1.409415	5.800913
H	1.274594	-2.676234	3.929723
H	1.043133	-1.873173	1.620346
H	1.654155	-1.830316	-0.557151
H	3.974259	-2.099467	-1.271264

H 5.404673 -0.108296 -1.668288

H 4.458961 2.159529 -1.314121

H 2.137406 2.433186 -0.548600

Cl 0.300759 3.081497 1.152885

Triphenylstibine 10

Zero-point correction = 0.272437 (Hartree/Particle)

Thermal correction to Energy = 0.289434

Thermal correction to Enthalpy = 0.290379

Thermal correction to Gibbs Free Energy = 0.223093

Sum of electronic and zero-point Energies = -934.702135

Sum of electronic and Thermal Energies= -934.685138

Sum of electronic and Thermal Enthalpies= -934.684194

Sum of electronic and Thermal Free Energies= -934.751479

C -2.091842 -1.622112 -0.329744

C -0.809386 -1.355315 -0.817963

C -0.287943 -2.176666 -1.820391

C -1.036448 -3.236500 -2.326019

C -2.314881 -3.485749 -1.838763

C -2.843771 -2.676295 -0.839046

Sb 0.258154 0.335461 -0.014312

C -0.489969 1.765122 -1.443149

C -1.267108 1.402896 -2.545988

C -1.697203 2.366725 -3.454442

C -1.353538 3.702051 -3.273572

C -0.582179 4.075114 -2.178023

C -0.159214 3.111975 -1.267275

C	2.106257	-0.060558	-1.049677
C	3.051333	-0.881364	-0.427307
C	4.245921	-1.203359	-1.064051
C	4.514668	-0.696928	-2.331174
C	3.586635	0.128383	-2.956910
C	2.388452	0.444046	-2.321350
H	2.858773	-1.279216	0.565191
H	4.966732	-1.844569	-0.570098
H	5.445968	-0.942305	-2.827914
H	3.793723	0.527240	-3.943327
H	1.671326	1.085522	-2.823451
H	-1.538984	0.363895	-2.702299
H	-2.300736	2.072486	-4.305424
H	-1.688360	4.450344	-3.982262
H	-0.313708	5.114711	-2.030090
H	0.436990	3.419927	-0.412788
H	0.706431	-1.990692	-2.213383
H	-0.619730	-3.866915	-3.103134
H	-2.896307	-4.310157	-2.234476
H	-3.838355	-2.867604	-0.453154
H	-2.515953	-1.002890	0.455821

Triphenylstibine complex with Cl^-, 10Cl

Zero-point correction = 0.272532 (Hartree/Particle)

Thermal correction to Energy = 0.291540

Thermal correction to Enthalpy = 0.292484

Thermal correction to Gibbs Free Energy = 0.222006

Sum of electronic and zero-point Energies = -1395.000718

Sum of electronic and Thermal Energies = -1394.981710

Sum of electronic and Thermal Enthalpies = -1394.980766

Sum of electronic and Thermal Free Energies = -1395.051244

C	2.118661	-0.436615	-2.459011
C	2.166924	-0.214709	-1.080908
C	3.405618	-0.290564	-0.440460
C	4.560766	-0.596534	-1.155584
C	4.497566	-0.818089	-2.527074
C	3.272521	-0.732436	-3.180219
Sb	0.379860	0.206824	0.078046
C	-0.421859	1.771329	-1.218719
C	-0.992003	1.489737	-2.464801
C	-1.513043	2.502207	-3.266838
C	-1.481107	3.821961	-2.831808
C	-0.921358	4.118143	-1.593626
C	-0.395070	3.105380	-0.795599
C	-0.774570	-1.363136	-1.036073
C	-2.173104	-1.267937	-1.063801
C	-2.972133	-2.284217	-1.578845
C	-2.385972	-3.446206	-2.073637
C	-1.002221	-3.575014	-2.042800
C	-0.212950	-2.546307	-1.528884
H	3.469634	-0.067985	0.619300
H	5.514016	-0.646201	-0.640308
H	5.398583	-1.048071	-3.085833

H	3.214056	-0.893308	-4.251694
H	1.168434	-0.381750	-2.981659
H	-1.043211	0.466504	-2.820907
H	-1.944530	2.255790	-4.231460
H	-1.887486	4.612866	-3.453415
H	-0.885109	5.145264	-1.245881
H	0.070219	3.352112	0.152748
H	0.866784	-2.668634	-1.524802
H	-0.533324	-4.476658	-2.424136
H	-3.002305	-4.242160	-2.477663
H	-4.051576	-2.171498	-1.595837
H	-2.654086	-0.366544	-0.687911
Cl	2.088264	2.261016	1.341276