Electronic Supplementary Material (ESI) for Chemical Communications.

Supporting Information

Reversing Lewis Acidity from Bismuth to Antimony

Deepti Sharma, [a] Selvakumar Balasubramaniam, [a] Sandeep Kumar, [b] Eluvathingal D. Jemmis *[b] and Ajay Venugopal *[a]

[a] School of Chemistry, Indian Institute of Science Education and Research Thiruvananthapuram, Vithura, Thiruvananthapuram 695551, India.

[b] Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore 560012, India

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1. Experimental Procedures

1.1 General Methods:

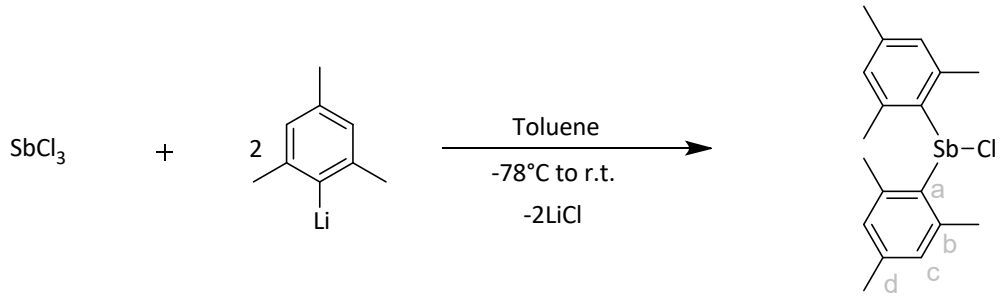
All the reaction procedures were carried out in argon atmosphere using standard glovebox and Schlenk line techniques. [1] All the glassware were dried at 200 °C before use. Dichloromethane, *n*-pentane, C_6D_5-Br and CD_2Cl_2 were dried over CaH_2. Na/Ph_2CO was used as a drying agent for toluene and diethyl ether (Et_2O).[2] The solvents were then distilled, degassed and stored over $LiAlH_4$ (toluene, *n*-pentane, Et_2O), CaH_2 (CH_2Cl_2, CD_2Cl_2) and 3 Å molecular sieves(C_6D_5-Br) at least a day prior to the use. Thereafter, the solvents were directly condensed into the reaction flask at -196 °C. Anhydrous $SbCl_3$, $BiCl_3$, Et_3PO and AgOTf were purchased from Sigma-Aldrich. $BiCl_3$, Et_3PO and AgOTf were directly taken into glovebox and used in experiments without any further purification. $SbCl_3$ was purified via sublimation and stored in glovebox. (Mesityl)Li, Tris(mesityl)bismuthine and $(Mesityl)_2BiCl$ were prepared according to the reported literature procedures.[3,4] $(Mesityl)_2SbCl$ was prepared by an alternative method to reported procedures.[5] 2-Bromomesitylene was procured from Sigma-Aldrich. It was dried over CaH_2 and stored over 3 Å molecular sieves before use.[2]

^1H, ^{13}C, ^{19}F and ^{31}P NMR spectra were recorded on Bruker Advance III 500 MHz spectrometer at ambient temperature. Chemical shifts (δ) are reported in ppm. ^1H and ^{13}C NMR spectra were referenced to the residual signals of the deuterated solvents. The chemical shifts (δ ppm) in ^1H and ^{13}C NMR spectra were referenced to the residual signals of the deuterated solvents. ^{19}F and ^{31}P NMR spectra were referenced to $CFCl_3$ and H_3PO_4 (85%) respectively. Abbreviations for NMR spectra: s (singlet), br (broad), m (multiplet). Percentage yields are reported for the crystallized products. Elemental analyses were performed on samples, well dried at 1×10^{-3} mbar at ambient temperature, on Elemental Vario Micro Cube instrument.

Synthesis and characterization of 1-Sb:

A 20 mL toluene solution of (Mesityl)Li (0.40 g, 3.17 mmol) was added dropwise to a 20 ml toluene solution of $SbCl_3$ (0.36 g, 1.58 mmol) at -78 °C. The reaction was allowed to attain ambient temperature and stirred for 15 h. The reaction mixture was filtered and toluene was distilled off. The yellow powder was dissolved in 2 mL *n*-pentane. Yellow crystals of **1-Sb** were obtained after 2 days at room temperature.

Yield: 0.37 g, 59 %



1-Sb

Scheme S1

Elemental analysis for $C_{18}H_{22}SbCl$ calculated: C, 54.65; H, 5.60; Found: C, 54.27; H, 5.60

^1H NMR (CD_2Cl_2, 500 MHz): δ 2.12 (s, 6H, *p*-CH_3), 2.64 (s, 12H, *o*-CH_3), 7.32 (s, 4H, C_6H_2)

$^{13}C\{^1H\}$ NMR (CD_2Cl_2, 125 MHz): δ 20.8 (*p*-CH_3), 24.7 (*o*-CH_3), 129.7 (c, C_9H_{11}), 139.8 (a, C_9H_{11}), 141.1 (d, C_9H_{11}), 143.8 (b, C_9H_{11})

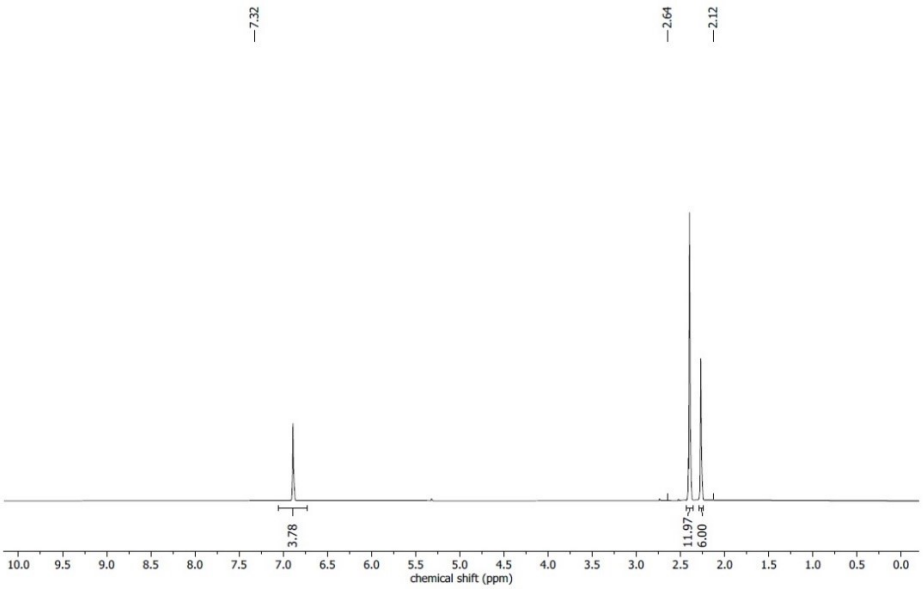


Figure S1: ^1H NMR spectrum of **1-Sb** in CD_2Cl_2.

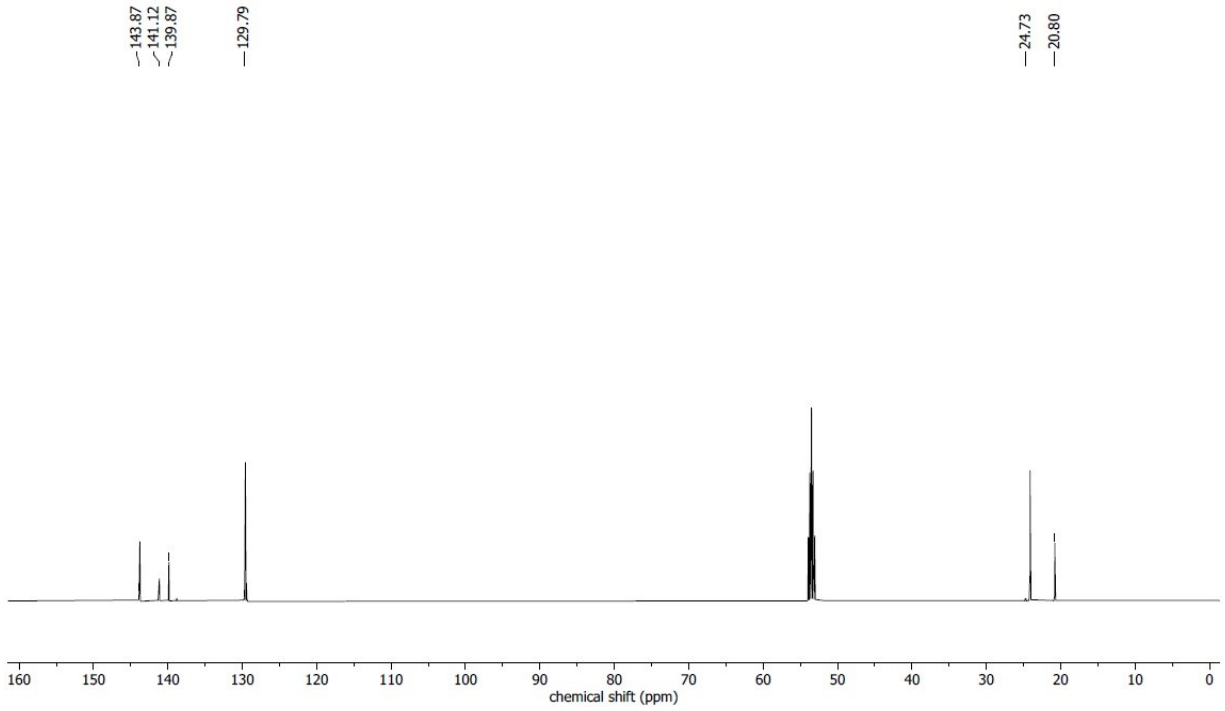
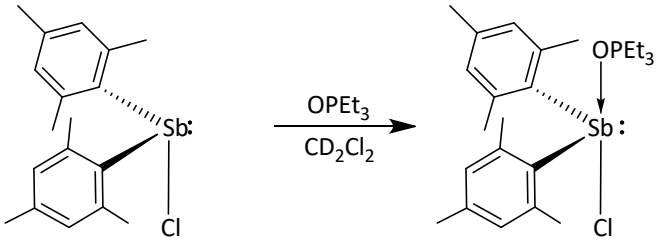


Figure S2: ^{13}C NMR spectrum of **1-Sb** in CD_2Cl_2.

Synthesis and characterization of 2-Sb:

1-Sb (0.011 g, 0.029 mmol) and Et_3PO (0.004 g, 0.029 mmol) were loaded in a J. Young NMR tube and 0.5 mL of CD_2Cl_2 was condensed on to the mixture. Quantitative conversion from **1-Sb** to **2-Sb** is confirmed by NMR spectroscopy after half an hour at ambient temperature.



1-Sb **2-Sb**

Scheme S2

^1H NMR (CD_2Cl_2, 500 MHz): δ 1.11 (m, 9H, $OPEt_3$, CH_3), 1.64 (m, 6H, $OPEt_3$, CH_2), 2.26 (s, 6H, *p*-CH_3), 2.40 (s, 12H,o-CH_3), 6.88 (s, 4H, C_6H_2)

^{31}P NMR (CD_2Cl_2, 202 MHz): δ 50.9 (s, $OPEt_3$)

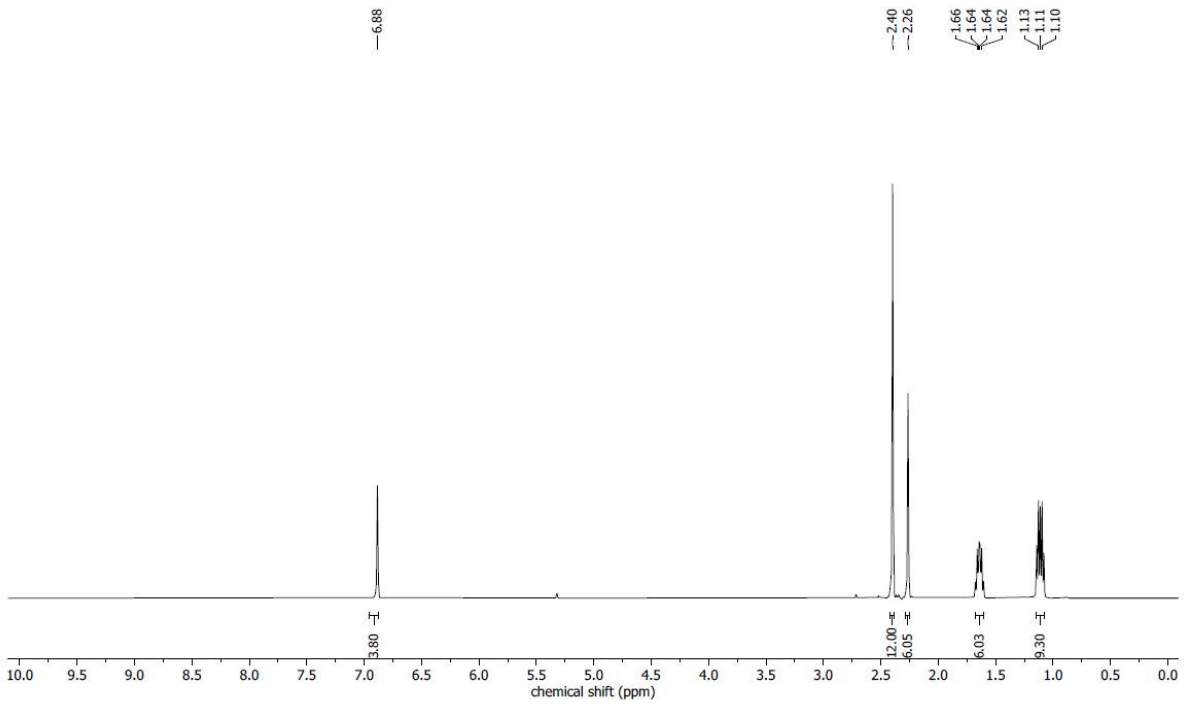


Figure S3: ^{1}H NMR spectrum of **2-Sb** in CD_2Cl_2.

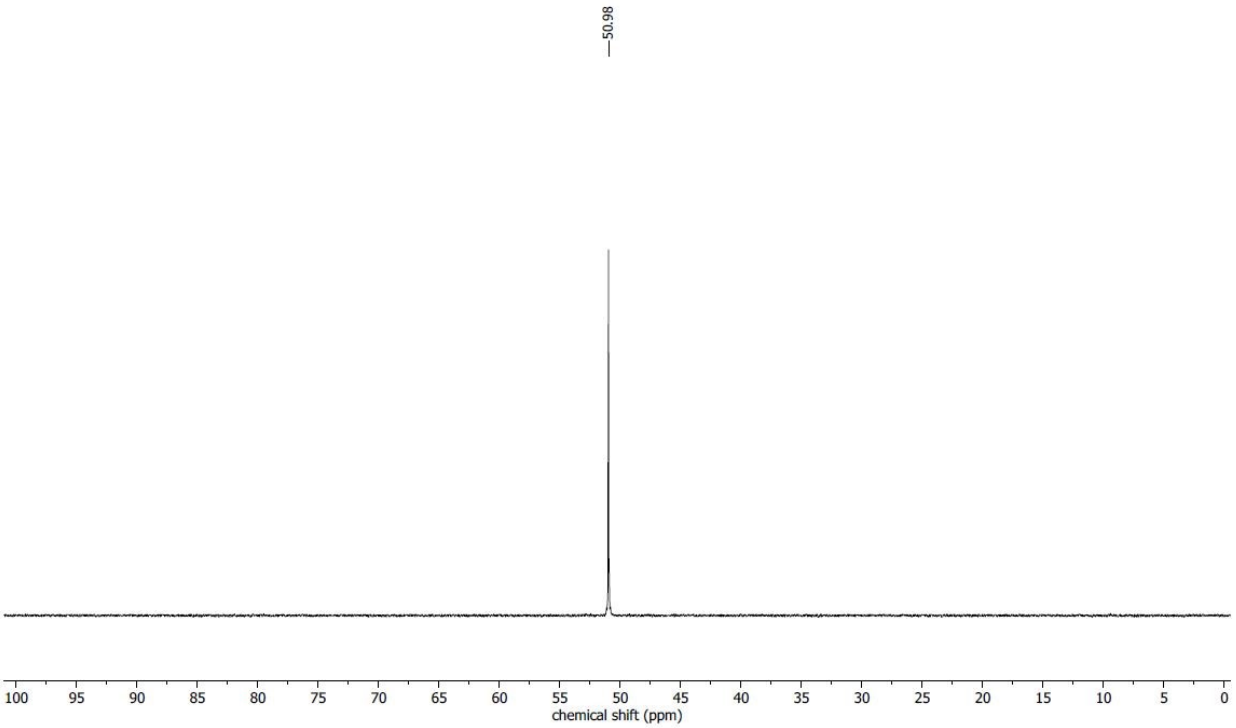
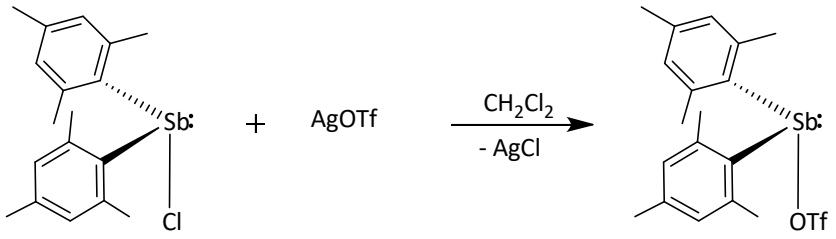


Figure S4: ^{31}P NMR spectrum of **2-Sb** in CD_2Cl_2.

Synthesis and Characterization of 3-Sb:

1-Sb (0.045 g, 0.11 mmol), and AgOTf (0.029 g, 0.11 mmol) were loaded into a Schlenk flask. Dichloromethane (10 mL) was condensed on to the mixture at -196 °C. The reaction mixture was allowed to attain room temperature and stirred overnight. Thereafter, filtration of reaction mixture gave a yellow solution. The solution was concentrated to 0.5 mL and stored at -30 °C. to receive yellow crystals together with yellow precipitate of **3-Sb**.

Yield: 0.027 g, 47 %



1-Sb **3-Sb**

Scheme S3

Elemental analysis for $C_{19}H_{22}F_3O_3SSb$ calculated: C, 44.81; H, 4.35; Found: C, 44.96; H, 4.27

^{1}H NMR (CD_2Cl_2, 500 MHz): δ 2.28 (s, 6H, p-CH_3), 2.35 (s, 12H, o-CH_3), 6.96 (s, 4H, C_6H_2)

^{1}H NMR (C_6D_5-Br, 500 MHz): δ 2.08 (s, 6H, *p*-CH_3), 2.25 (s, 12H, *o*-CH_3), 6.69 (s, 4H, C_6H_2)

^{13}C{^{1}H} NMR (C_6D_5-Br, 125 MHz): δ 21.0 (*p*-CH_3), 23.4 (*o*-CH_3), 122.1 (c, C_9H_{11}), 130.0 (a, C_9H_{11}), 140.8 (d, C_9H_{11}), 142.9 (b, C_9H_{11})

^{19}F NMR (CD_2Cl_2, 470 MHz): δ -77.6 (s, 3F, SO_3CF_3)

^{19}F NMR (C_6D_5-Br, 470 MHz): δ -76.6 (s, 3F, SO_3CF_3)

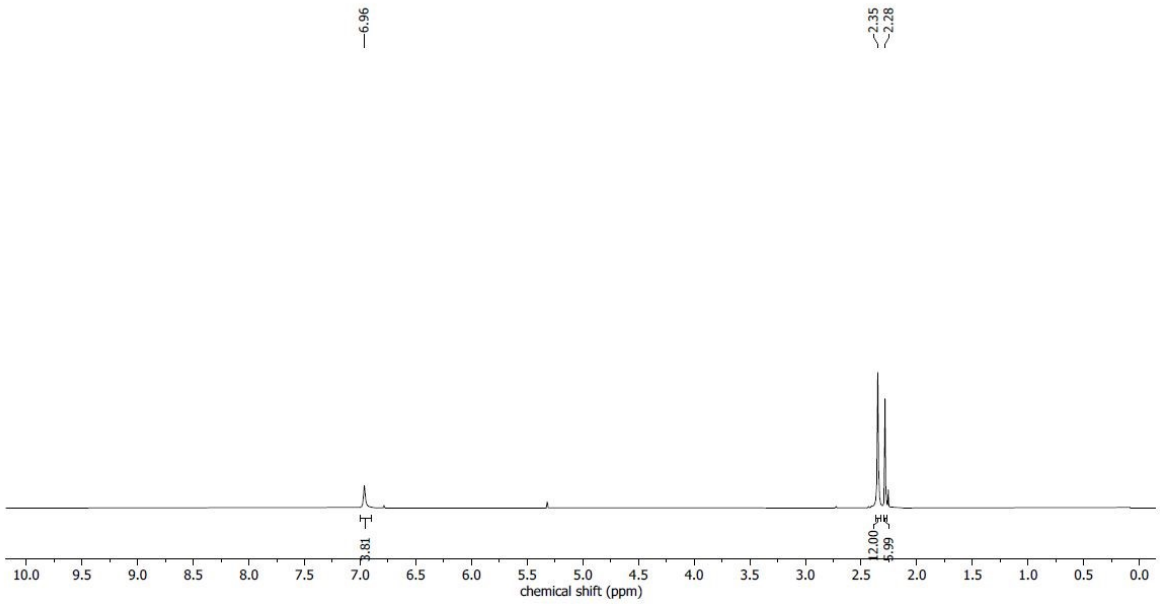


Figure S5: ^{1}H NMR spectrum of **3-Sb** in CD_2Cl_2.

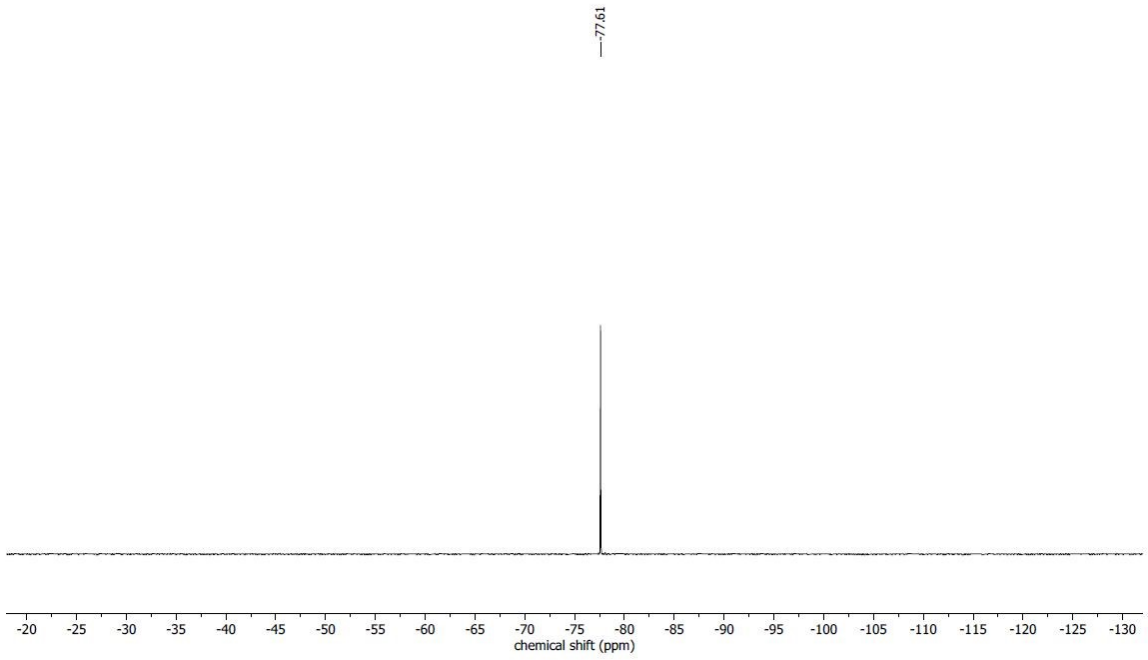


Figure S6: ^{19}F NMR spectrum of **3-Sb** in CD_2Cl_2.

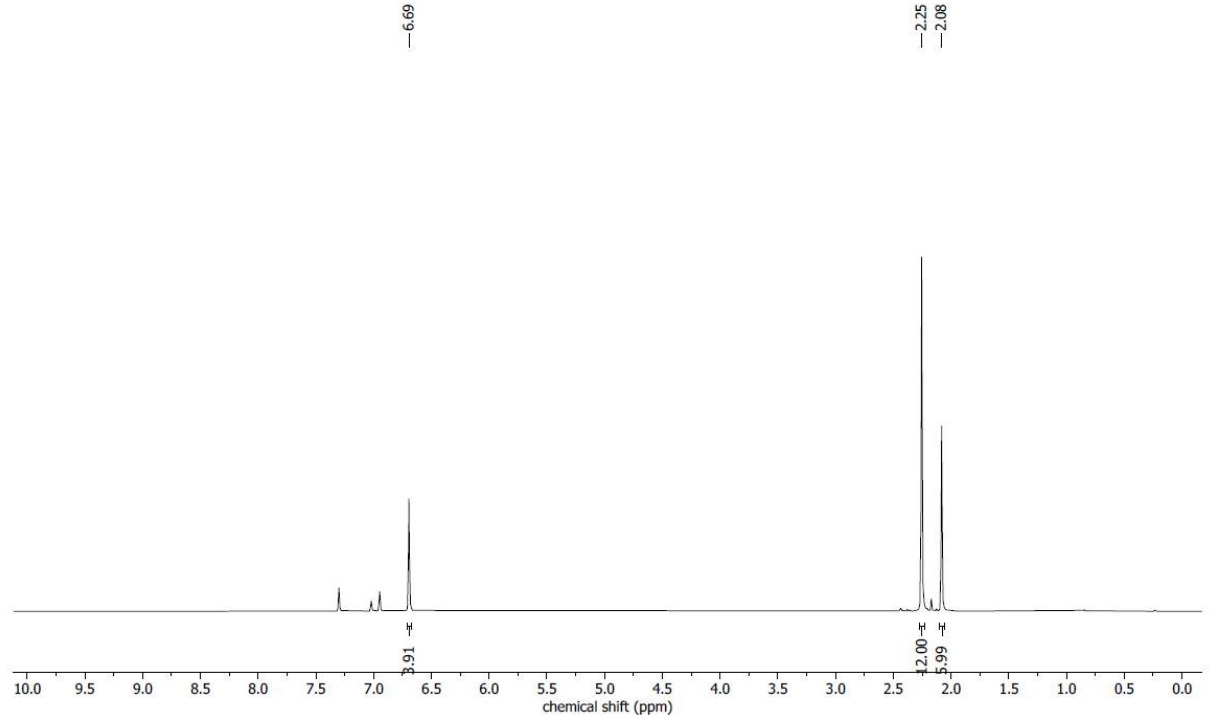


Figure S7: ^{1}H NMR spectrum of **3-Sb** in C_6D_5-Br.

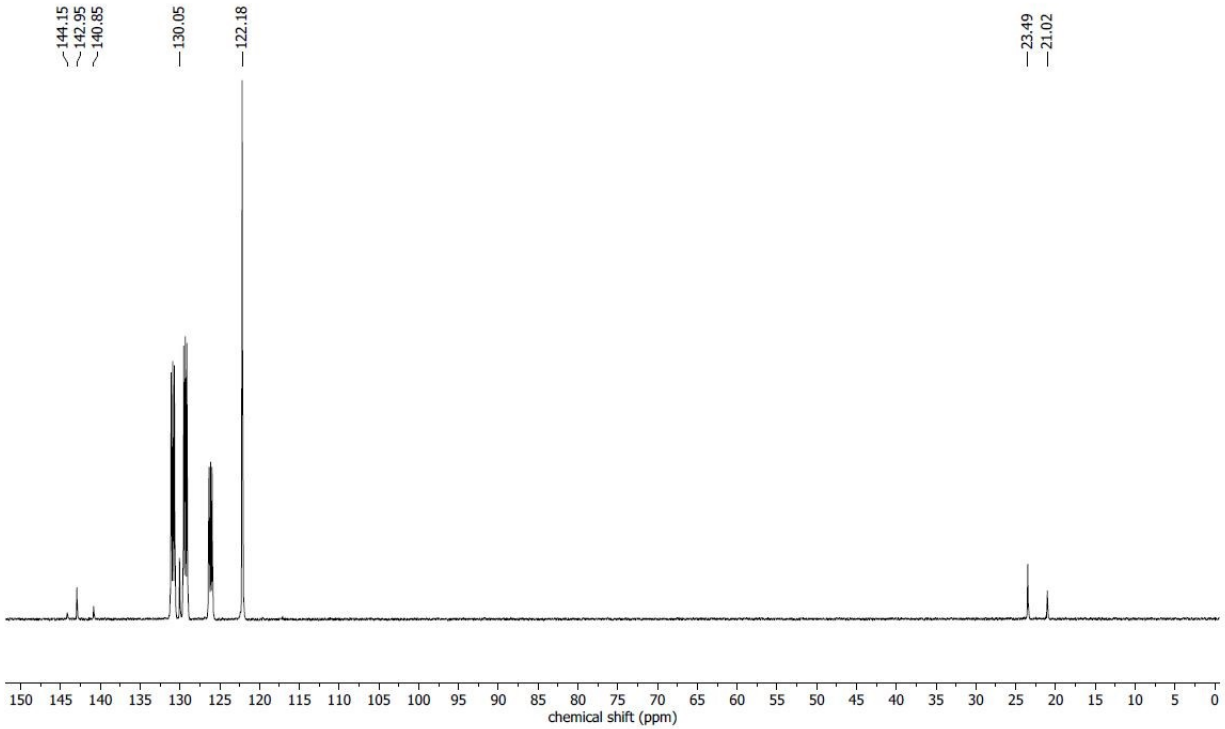


Figure S8: ^{13}C NMR spectrum of **3-Sb** in C_6D_5-Br.

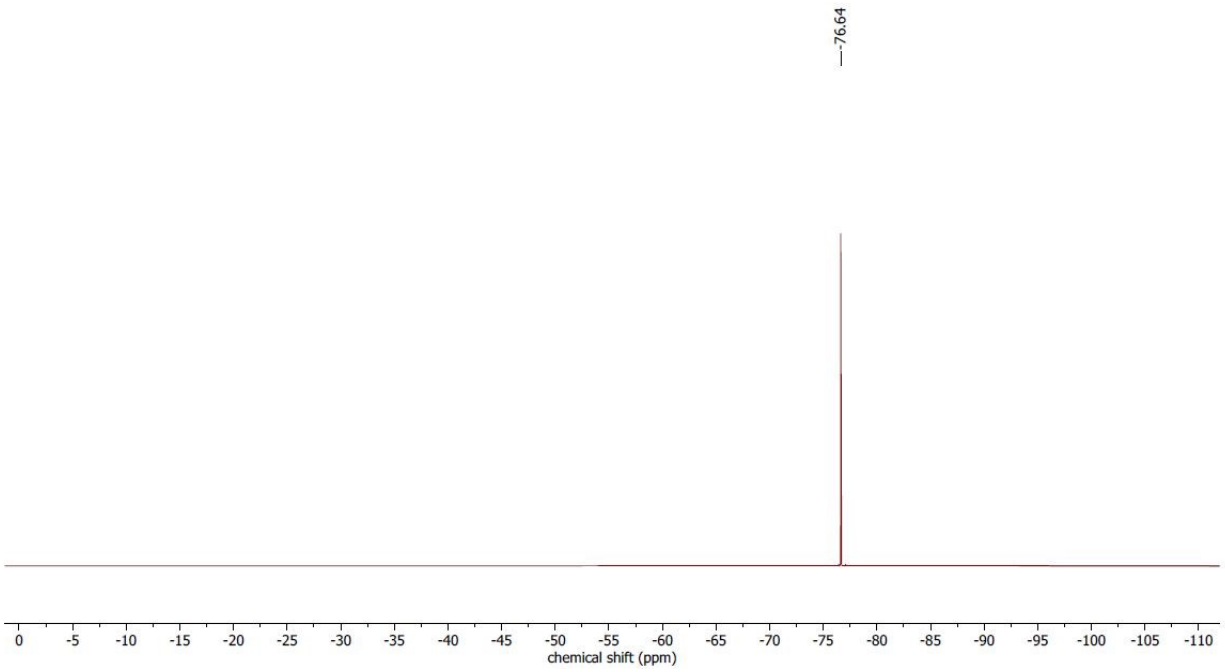
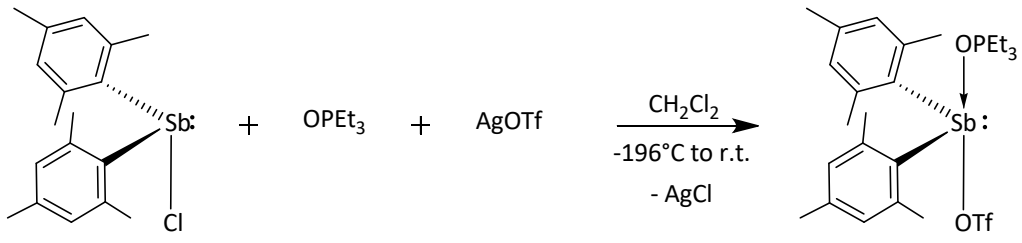


Figure S9: ^{19}F NMR spectrum of **3-Sb** in C_6D_5-Br.

Synthesis and characterization of 4-Sb:

1-Sb (0.045 g, 0.11 mmol), O=PEt_3 (0.015 g, 0.11 mmol) and AgOTf (0.029 g, 0.11 mmol) were loaded into a Schlenk flask. Dichloromethane (10 mL) was condensed onto the mixture at -196 °C. The reaction mixture was allowed to attain room temperature and stirred for 2 h. Thereafter, filtration of reaction mixture gave a colorless solution. The solution was concentrated to 1.5 mL, layered with n-pentane and stored at -30 °C to obtain colorless crystals of **4-Sb**.

Yield: 0.046 g, 63 %



1-Sb **4-Sb**

Scheme S4

Elemental analysis for $C_{25}H_{37}F_3O_4PSSb$ calculated: C, 46.67; H, 5.80; Found: C, 46.29; H, 5.92

^1H NMR (CD_2Cl_2, 500 MHz): δ 1.08 (m, 9H, $OPEt_3$, CH_3), 1.87 (m, 6H, $OPEt_3$, CH_2), 2.28 (s, 6H, *p*-CH_3), 2.40 (s, 12H, o-CH_3), 6.95 (s, 4H, C_6H_2)

^{1}H NMR (C_6D_5-Br, 500 MHz): δ 0.70 (m, 9H, $OPEt_3$, CH_3), 1.42 (m, 6H, $OPEt_3$, CH_2), 2.13 (s, 6H, *p*-CH_3), 2.48 (s, 12H, *o*-CH_3), 6.80 (s, 4H, C_6H_2)

^{13}C{^{1}H} NMR (C_6D_5-Br, 125 MHz): δ 4.9 (d, $^{2}J_{CP}$=5.35 Hz, OPEt3, CH_3), 17.8 (d, , $^{1}J_{CP}$=64.14 Hz, $OPEt_3$, CH_2), 20.9 (p-CH_3), 24.2 (o-CH_3), 122.1 (c, C_9H_{11}), 126.9 (a, C_9H_{11}), 139.2 (d, C_9H_{11}), 143.8 (b, C_9H_{11})

^{19}F NMR (CD_2Cl_2, 470 MHz): δ -78.9 (s, 3F, SO_3CF_3)

^{19}F NMR (C_6D_5-Br, 470 MHz): δ -77.3 (s, 3F, SO_3CF_3)

^{31}P NMR (CD_2Cl_2, 202 MHz): δ 81.6 (s, br, $OPEt_3$)

^{31}P NMR (C_6D_5-Br, 202 MHz): δ 72.8 (s, br, $OPEt_3$)

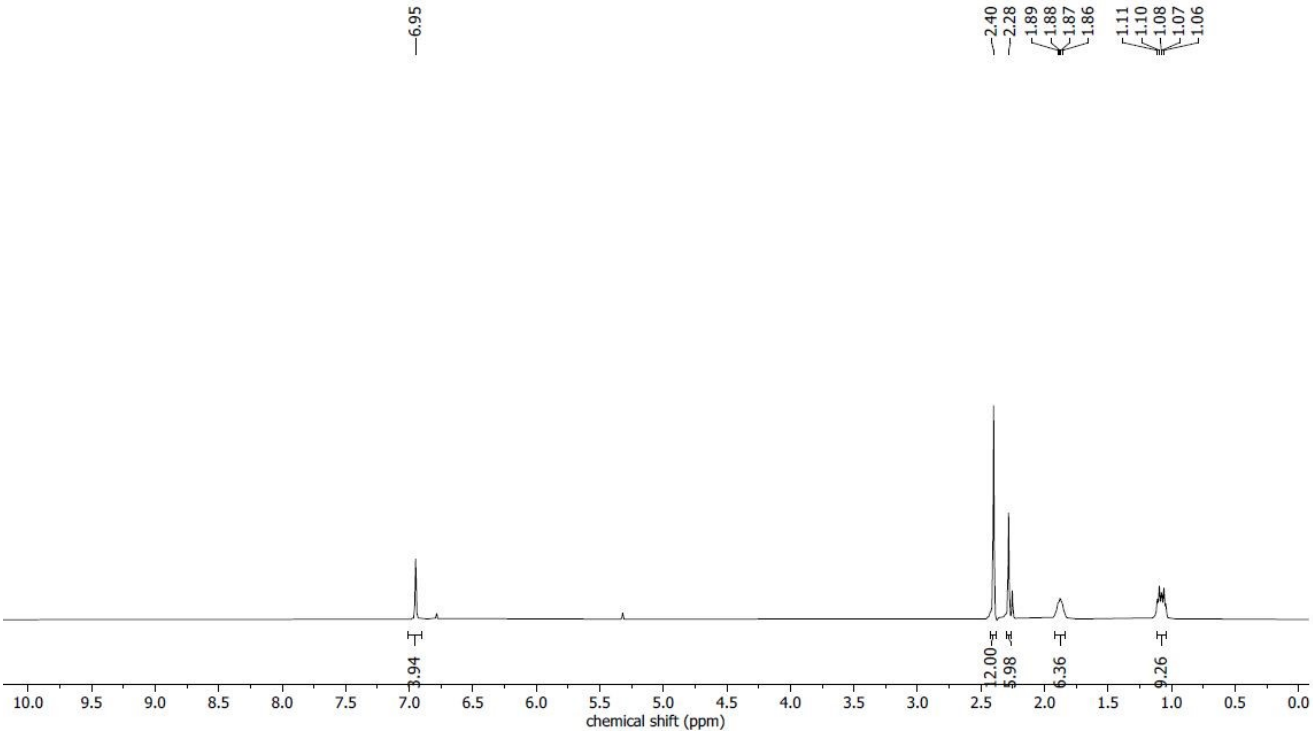


Figure S10: ^{1}H NMR spectrum of **4-Sb** in CD_2Cl_2.

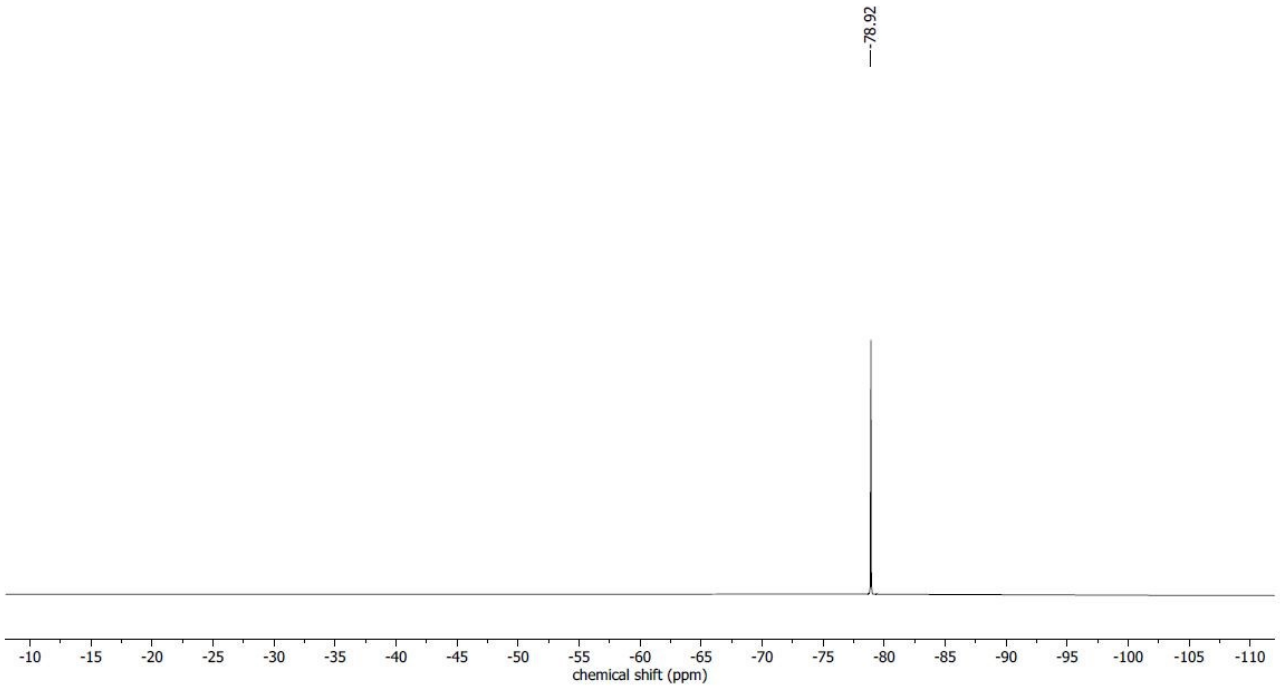


Figure S11: ^{19}F NMR spectrum of **4-Sb** in CD_2Cl_2.

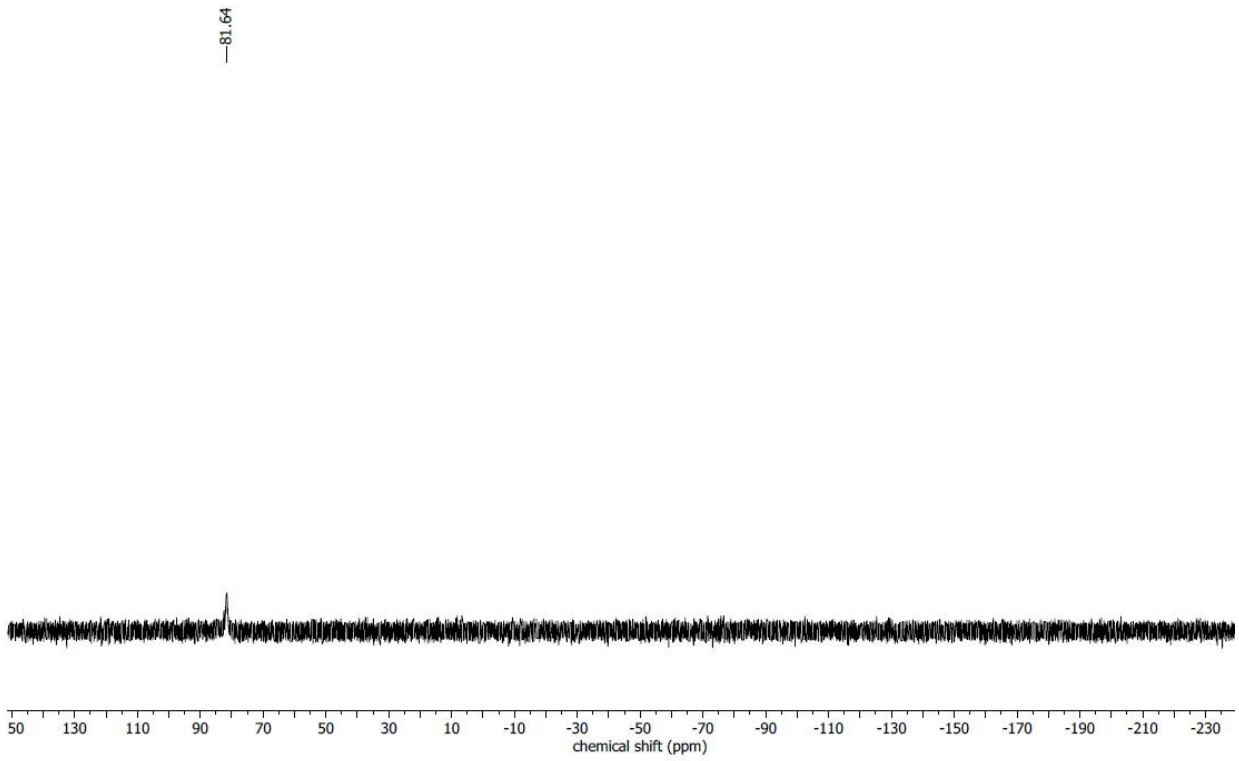


Figure S12: ^{31}P NMR spectrum of **4-Sb** in CD_2Cl_2.

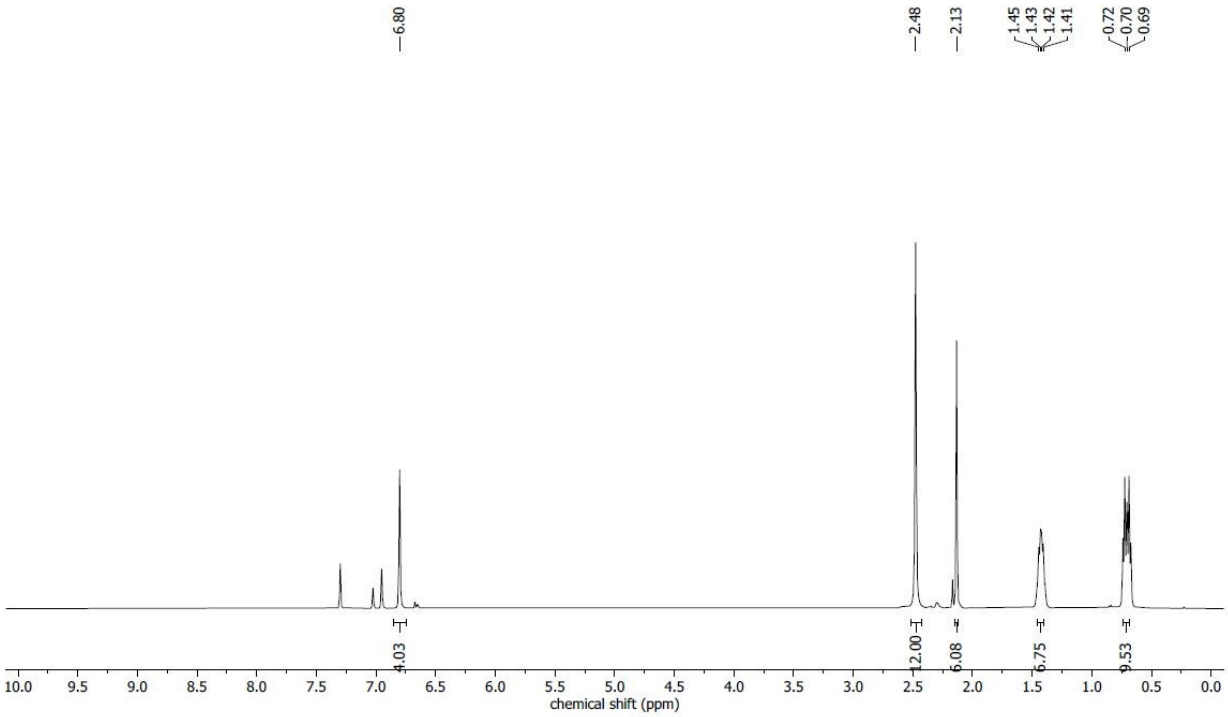


Figure S13: ^{1}H NMR spectrum of **4-Sb** in C_6D_5-Br.

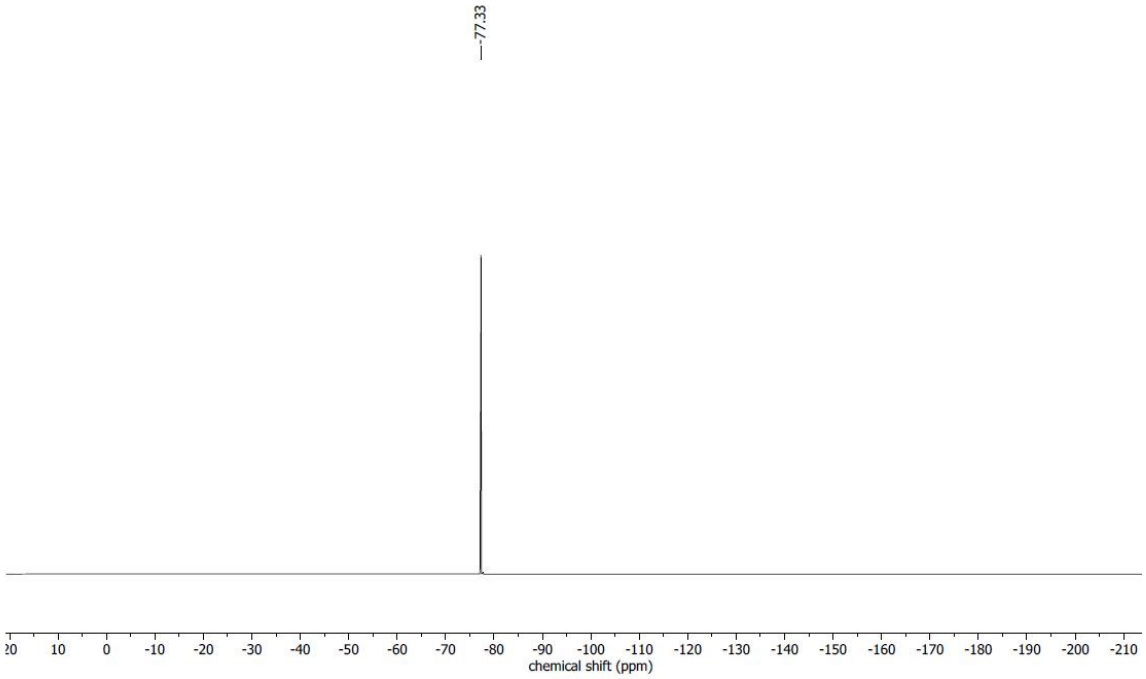


Figure S14: ^{19}F NMR spectrum of **4-Sb** in C_6D_5-Br.

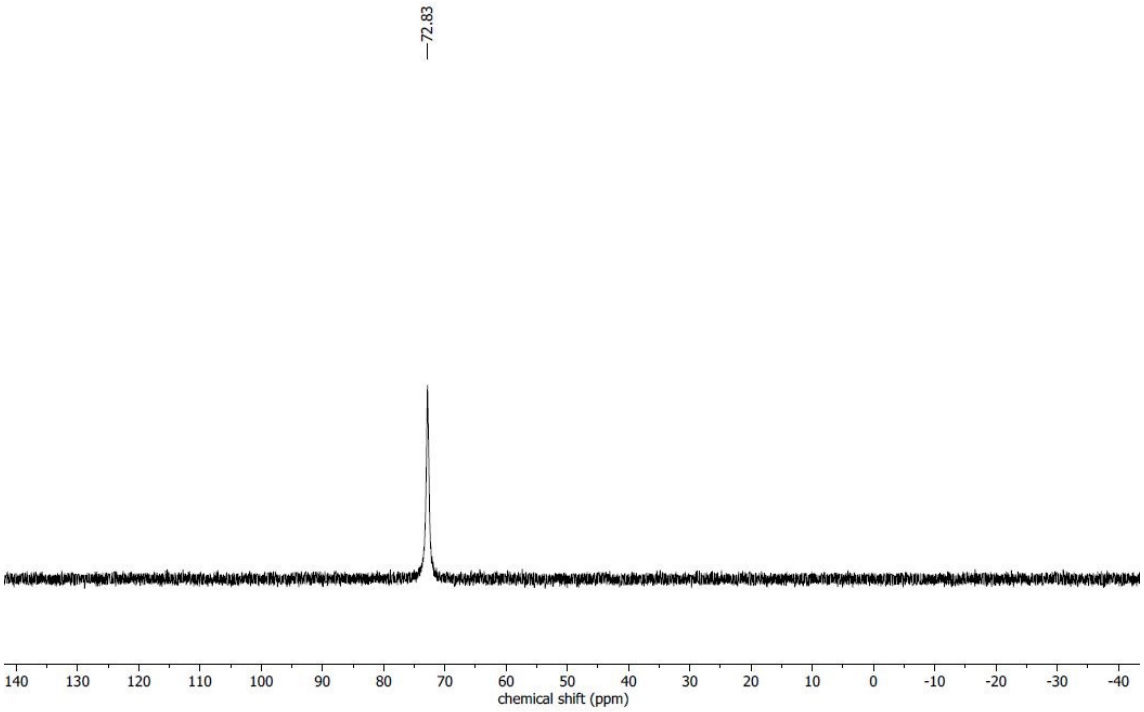


Figure S15: ^{31}P NMR spectrum of **4-Sb** in C_6D_5-Br.

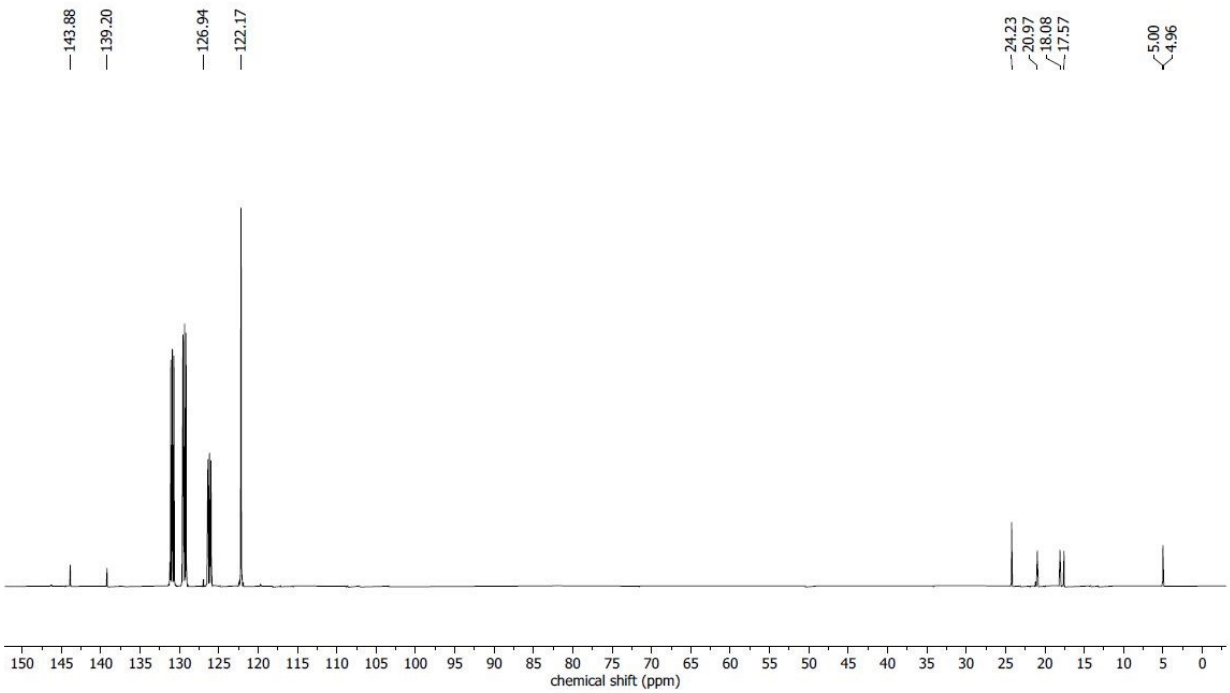


Figure S16: ^{13}C NMR spectrum of **4-Sb** in C_6D_5-Br.

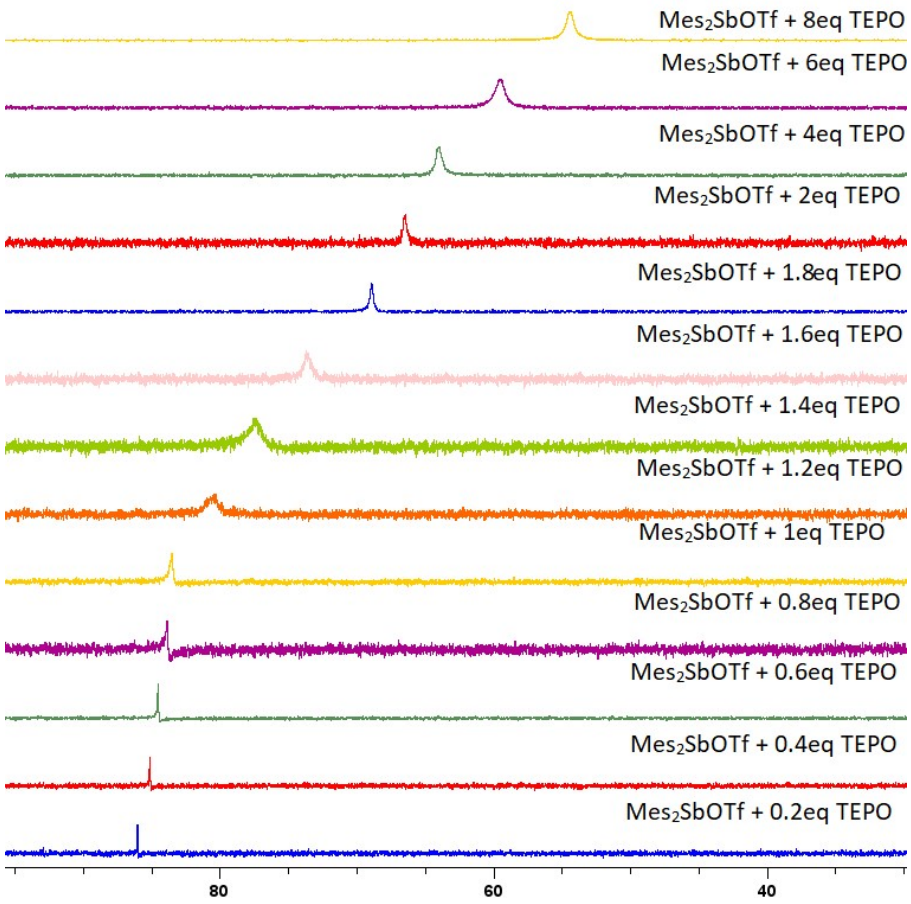
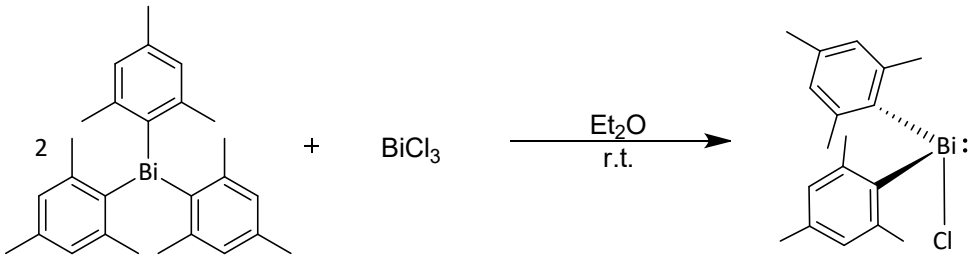


Figure S17: Stacked ^{31}P NMR spectra of **3-Sb** in CD_2Cl_2 with varying concentration of Et_3PO.

Synthesis of 1-Bi:

$(Mesityl)_3Bi$ (0.4 g, 0.70 mmol) and $BiCl_3$(0.11 g, 0.35 mmol) were loaded into a Schlenk flask and diethyl ether (40 mL) is condensed over the reaction mixture at -196 °C. The reaction was allowed to reach an ambient temperature and left on stirring for 16 h. Thereafter, diethyl ether was distilled off completely and yellowish green solid is washed with *n*-pentane to receive **1-Bi**.

Yield: 0.44 g, 86 %



1-Bi

Scheme S5

Elemental analysis for $C_{18}H_{22}BiCl$ calculated: C, 44.77; H, 4.59; Found: C, 44.91; H, 4.63

^{1}H NMR (C_6D_5-Br), 500 MHz): δ 2.11 (s, 6H, *p*-CH_3), 2.30 (s, 12H, *o*-CH_3), 7.02 (s, 4H, C_6H_2)

$^{13}C\{^{1}H\}$ NMR (C_6D_5-Br), 125 MHz): δ 21.1 (*p*-CH_3), 25.4 (*o*-CH_3), 122.1 (c, C_9H_{11}), 131.9 (a, C_9H_{11}), 138.1 (d, C_9H_{11}), 145.3 (b, C_9H_{11})

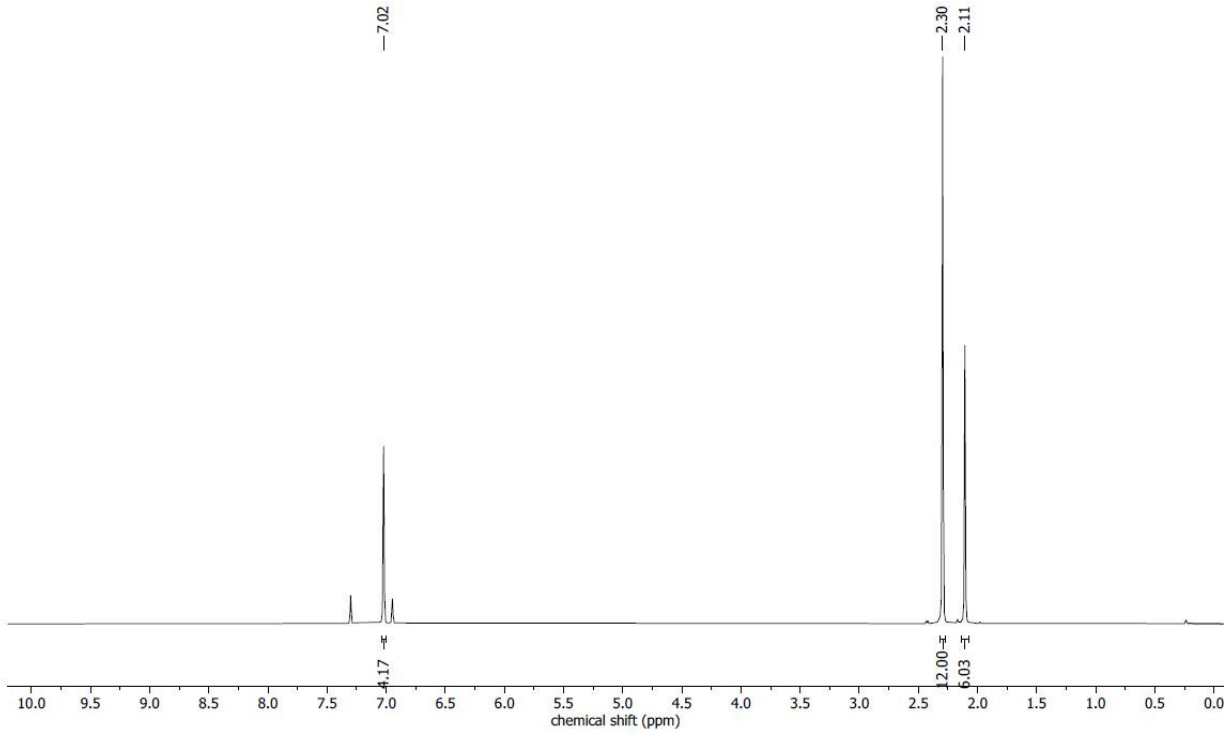


Figure S18: ^{1}H NMR spectrum of **1-Bi** in C_6D_5-Br.

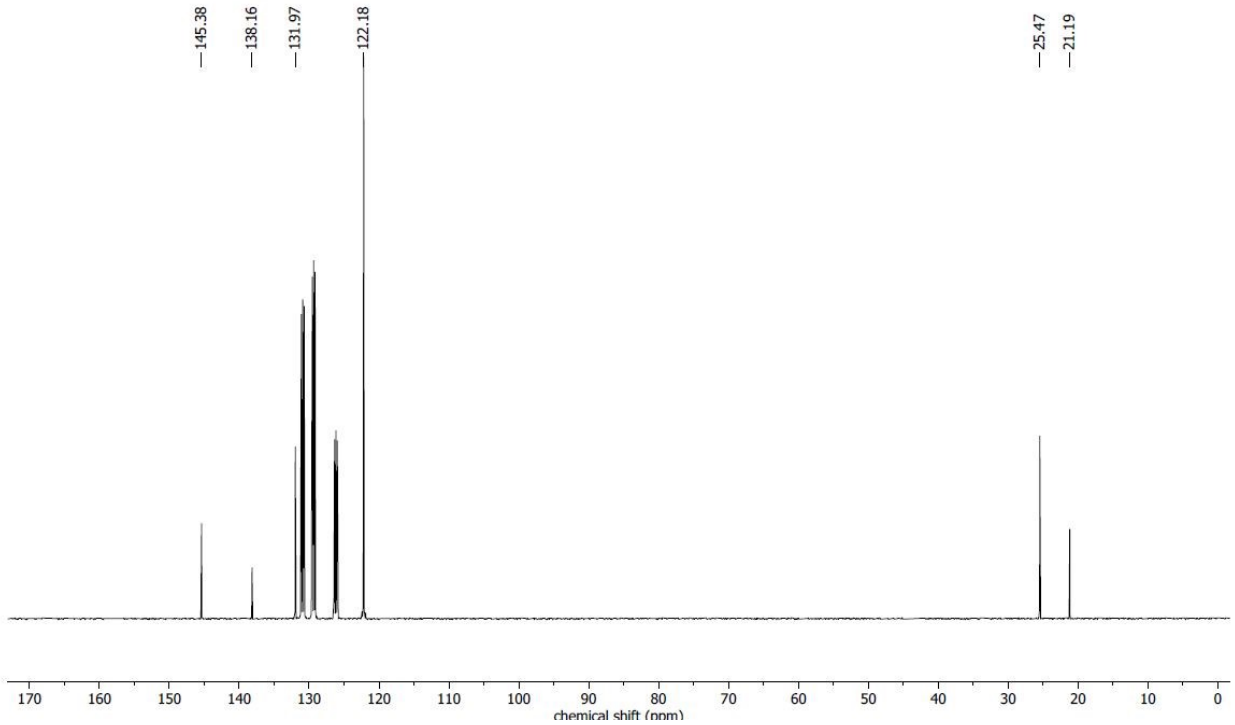
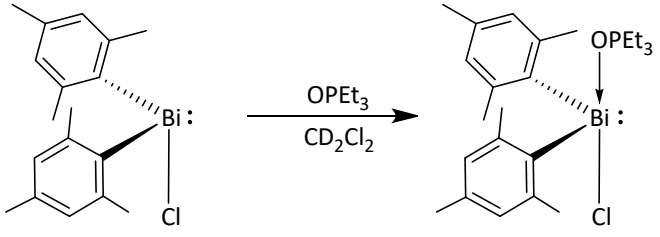


Figure S19: ^{13}C NMR spectrum of **1-Bi** in C_6D_5-Br.

Synthesis and characterization of 2-Bi:

1-Bi (0.014 g, 0.029 mmol) and Et_3PO (0.004 g, 0.029 mmol) were loaded in a J. Young NMR tube and 0.5 mL of CD_2Cl_2 was condensed onto the mixture. Quantitative conversion from **1-Bi** to **2-Bi** was confirmed by NMR spectroscopy after half an hour.



1-Bi **2-Bi**

Scheme S6

^1H NMR (CD_2Cl_2, 500 MHz): δ 1.02 (m, 9H, $OPEt_3$, CH_3), 1.55 (m, 6H, $OPEt_3$, CH_2), 2.25 (s, 6H, *p*-CH_3), 2.43 (s, 12H, *o*-CH_3), 7.22 (s, 4H, C_6H_2)

^{31}P NMR (CD_2Cl_2, 202 MHz): δ 55.2 (s, br, $OPEt_3$)

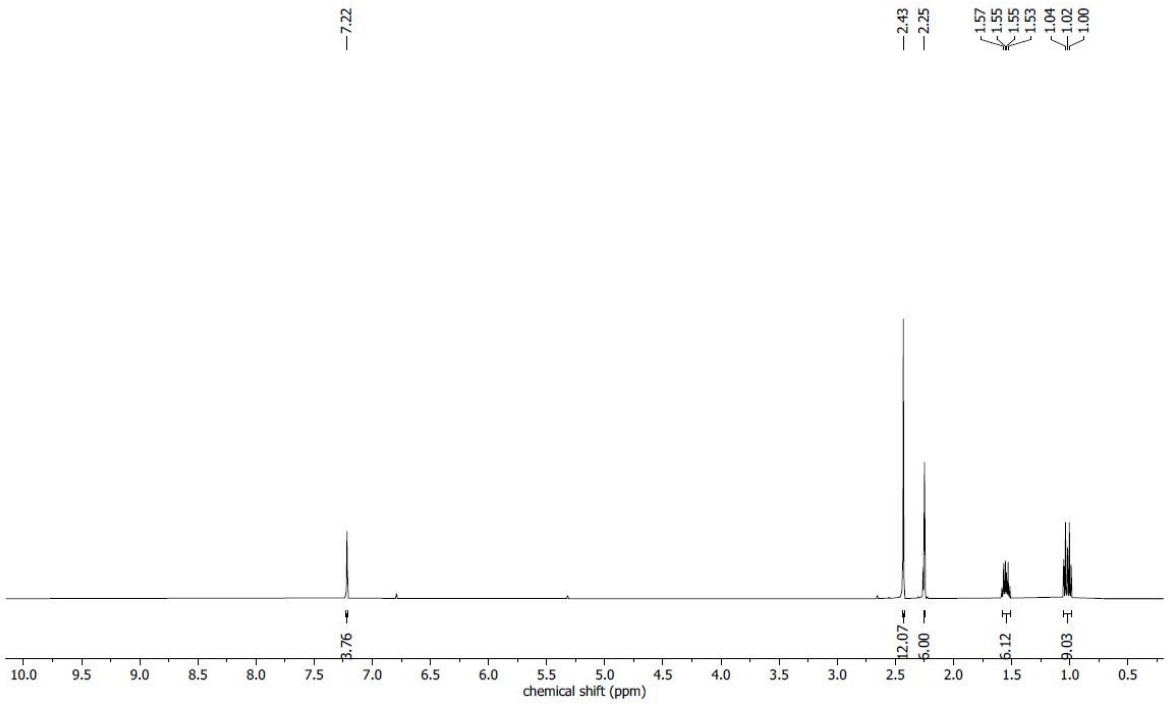


Figure S20: ^{1}H NMR spectrum of **2-Bi** in CD_2Cl_2.

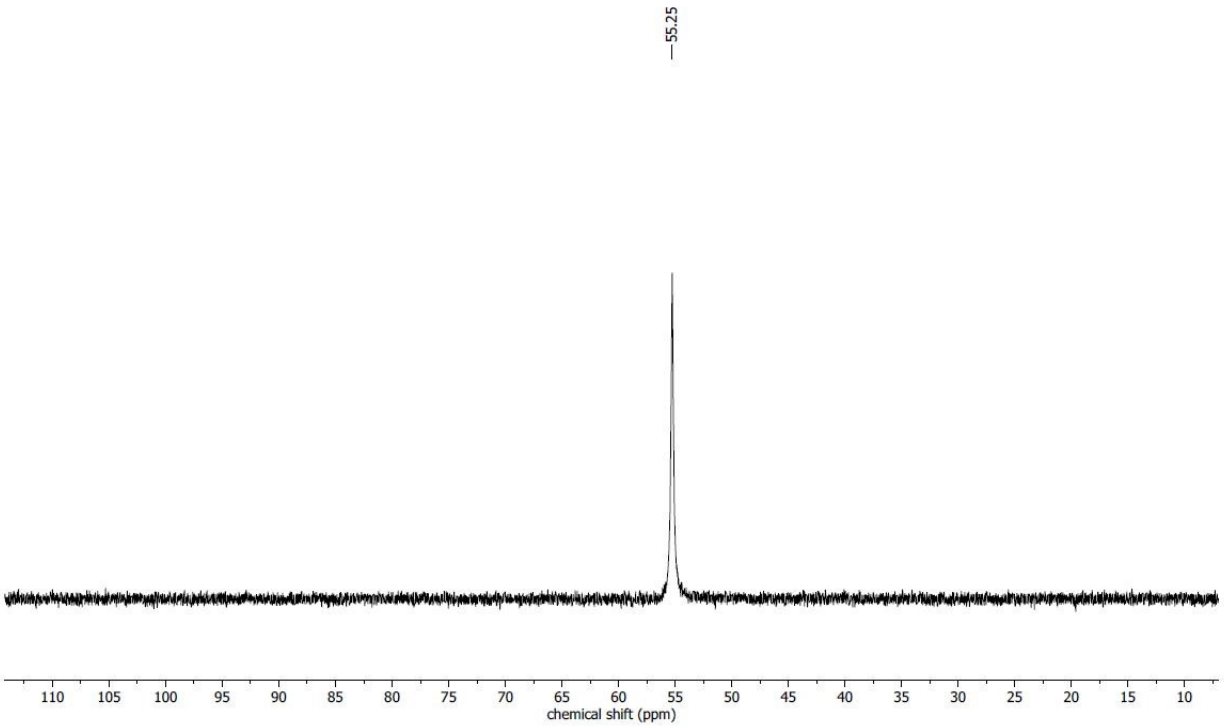
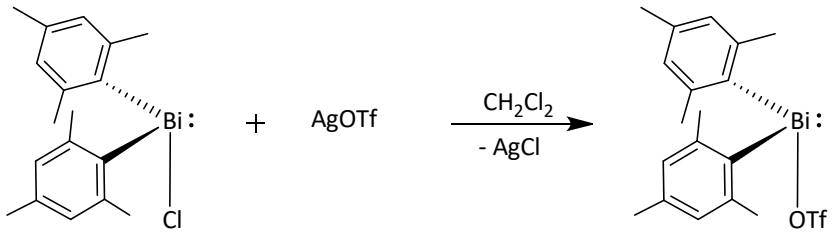


Figure S21: ^{31}P NMR spectrum of **2-Bi** in CD_2Cl_2.

Synthesis of 3-Bi:

1-Bi (0.045 g, 0.09 mmol), and AgOTf (0.023 g, 0.09 mmol) were loaded into a Schlenk flask. Dichloromethane (10 mL) was condensed onto the mixture at -196 °C. The reaction mixture was allowed to attain room temperature and stirred overnight. Thereafter, filtration of reaction mixture gave a dark yellow solution. The solution was concentrated to 0.5 mL and stored over -30 °C to receive yellow precipitate of **3-Bi**.

Yield: 0.023 g, 42 %



1-Bi **3-Bi**

Scheme S7

Elemental analysis for $C_{19}H_{22}F_3O_3SBi$ calculated: C, 38.26; H, 3.72; Found: C, 37.98; H, 3.78

^{1}H NMR (C_6D_5-Br, 500 MHz): δ 2.06 (s, 6H, *p*-CH_3), 2.18 (s, 12H,*o*-CH_3), 7.22 (s, 4H, C_6H_2)

^{19}F NMR (CD_2Cl_2, 470 MHz): δ -77.8 (s, 3F, SO_3CF_3)

^{19}F NMR (C_6D_5-Br, 470 MHz): δ -76.4 (s, 3F, SO_3CF_3)

Due to the poor solubility of **3-Bi** in CD_2Cl_2 and C_6D_5-Br, ^{13}C NMR spectrum could not be obtained.

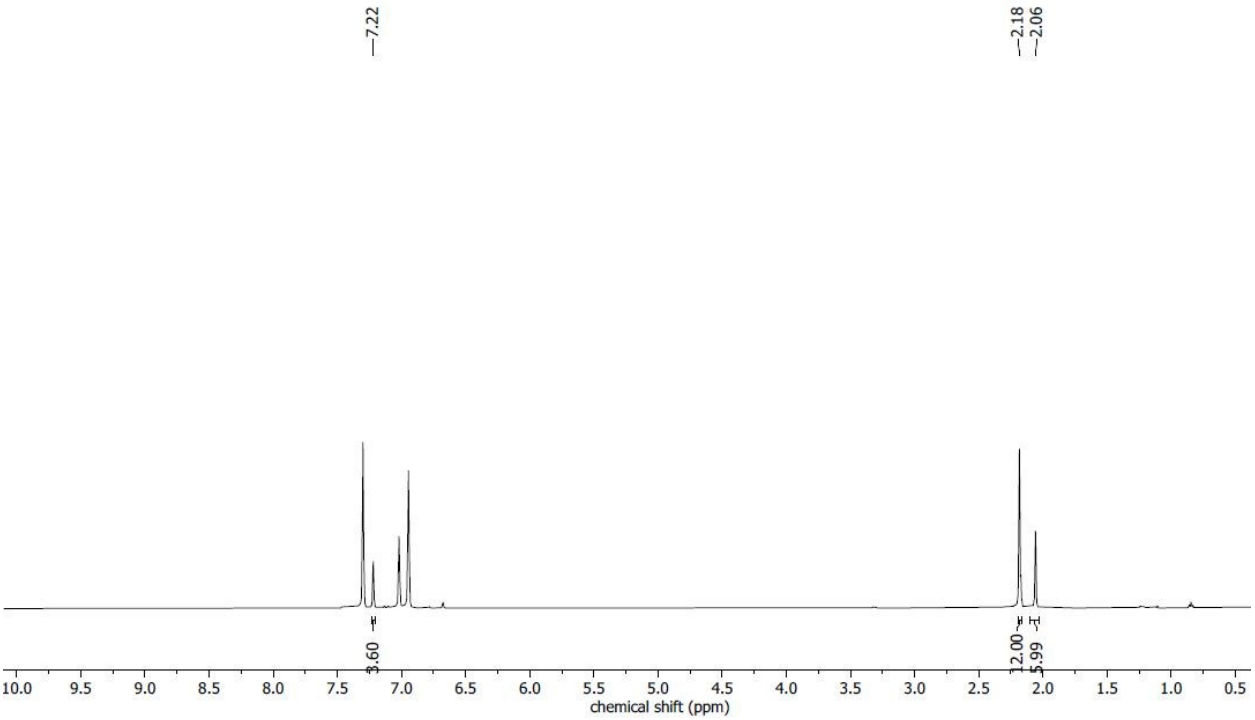


Figure S22: ^{1}H NMR spectrum of **3-Bi** in C_6D_5-Br.

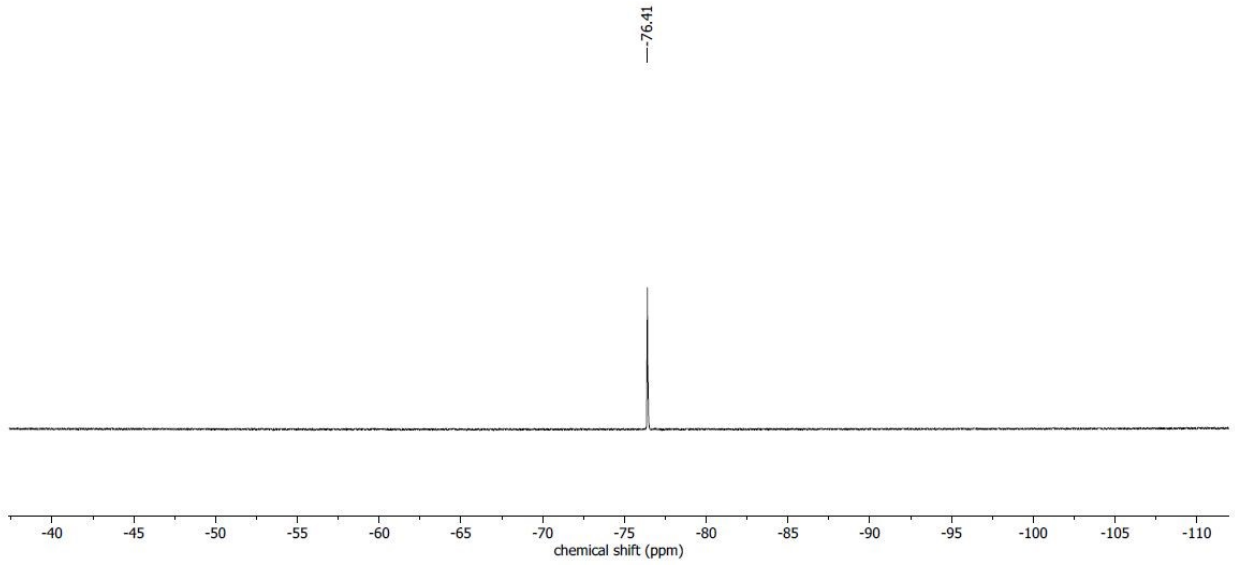


Figure S23: ^{19}F NMR spectrum of **3-Bi** in C_6D_5-Br.

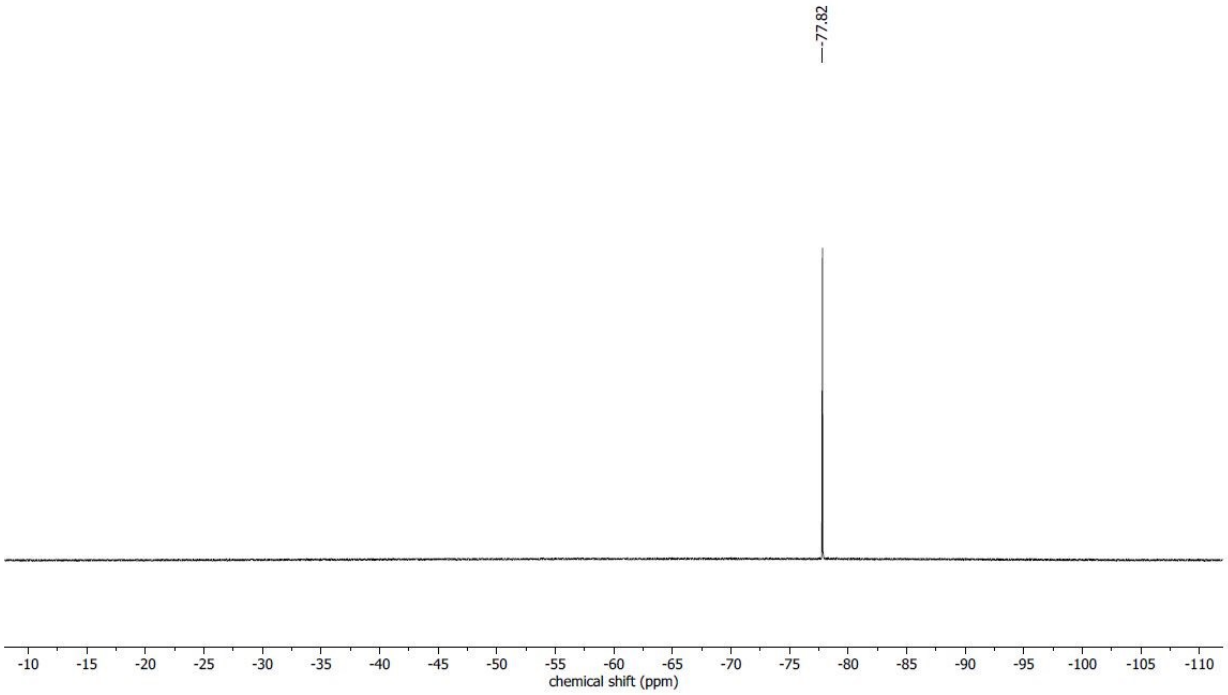
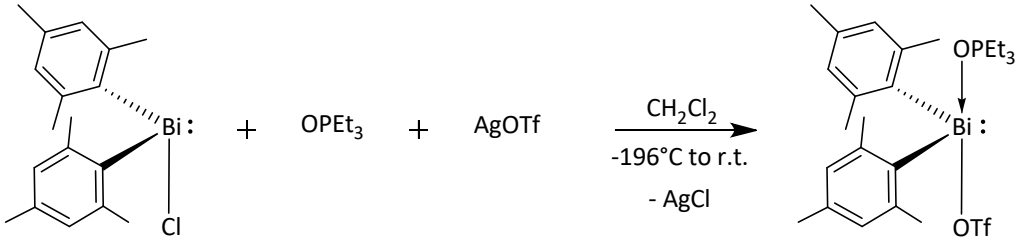


Figure S24: ^{19}F NMR spectrum of **3-Bi** in CD_2Cl_2.

Synthesis and characterization of 4-Bi:

1-Bi (0.045 g, 0.09 mmol), Et_3PO (0.012 g, 0.09 mmol) and AgOTf (0.023 g, 0.09 mmol) were loaded into a Schlenk flask. Dichloromethane (5 mL) was condensed onto the mixture at -196 °C. The reaction mixture was allowed to attain room temperature and stirred for 4 h. Thereafter, filtration of reaction mixture gave a pale-yellow solution. The solution was concentrated to 1 mL, layered with *n*-pentane and stored over -30 °C to obtain colorless crystals of **4-Bi**.

Yield: 0.038 g, 56 %



1-Bi **4-Bi**

Scheme S8

Elemental analysis for $C_{25}H_{37}F_3O_4PSBi$ calculated: C, 41.10; H, 5.10; Found: C, 41.34; H, 5.02

^{1}H NMR (CD_2Cl_2, 500 MHz): δ 1.00(m, 9H, $OPEt_3$, CH_3), 1.63(m, 6H, $OPEt_3$, CH_2),2.25 (s, 6H, *p*-CH_3), 2.40 (s, 12H, *o*-CH_3), 7.27 (s, 4H, C_6H_2)

^{1}H NMR (C_6D_5-Br, 500 MHz): δ 0.57 (m, 9H, $OPEt_3$, CH_3), 1.08 (m, 6H, $OPEt_3$, CH_2), 2.11 (s, 6H, *p*-CH_3), 2.49 (s, 12H,*o*-CH_3), 7.19 (s, 4H, C_6H_2)

^{13}C{^{1}H} NMR (C_6D_5-Br, 125 MHz): δ 5.0 (d, $^{1}J_{CP}$=5.16 Hz, $OPEt_3$, CH_3), 17.9 (d, $^{1}J_{CP}$=65.33 Hz $OPEt_3$, CH_2), 21.3 (*p*-CH_3), 25.9 (*o*-CH_3), 122.1 (c, C_9H_{11}), 131.8 (a, C_9H_{11}), 138.4 (d, C_9H_{11}), 146.3 (b, C_9H_{11})

^{19}F NMR (CD_2Cl_2, 470 MHz): δ -78.7 (s, 3F, SO_3CF_3)

^{19}F NMR (C_6D_5-Br, 470 MHz): δ -77.3 (s, 3F, SO_3CF_3)

^{31}P NMR (CD_2Cl_2, 202 MHz): δ 64.6 (s, br, $OPEt_3$)

^{31}P NMR (C_6D_5-Br, 202 MHz): δ 65.2 (s, br, $OPEt_3$)

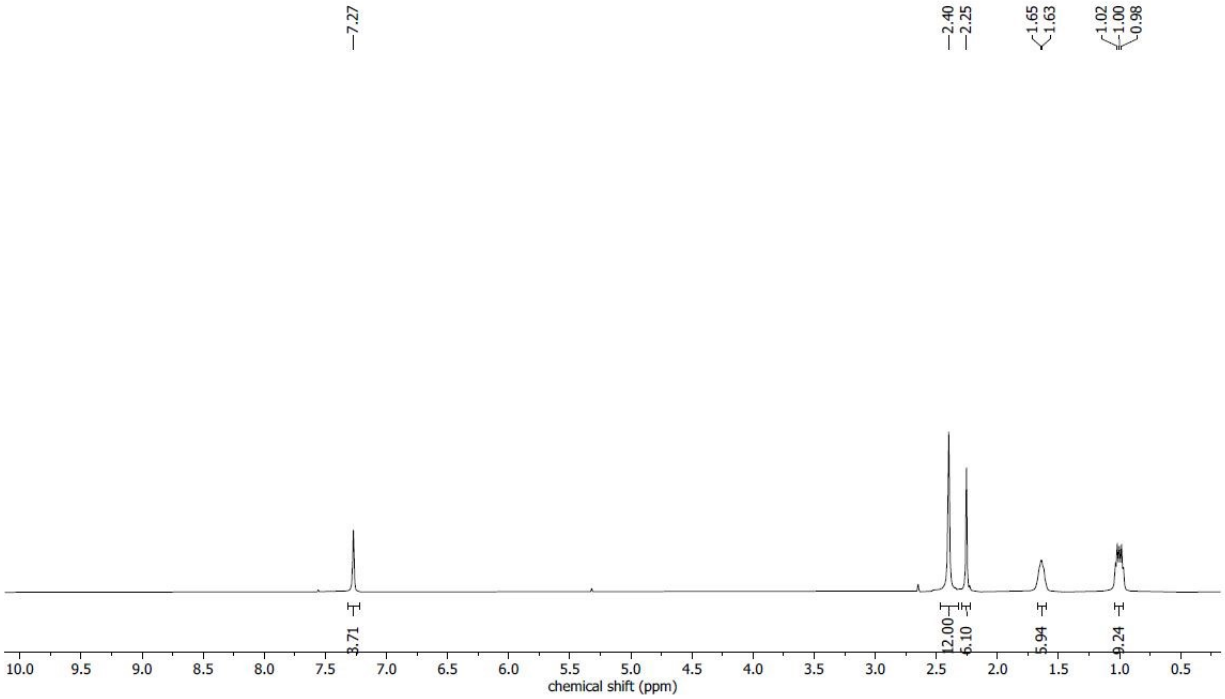


Figure S25: ^{1}H NMR spectrum of **4-Bi** in CD_2Cl_2.

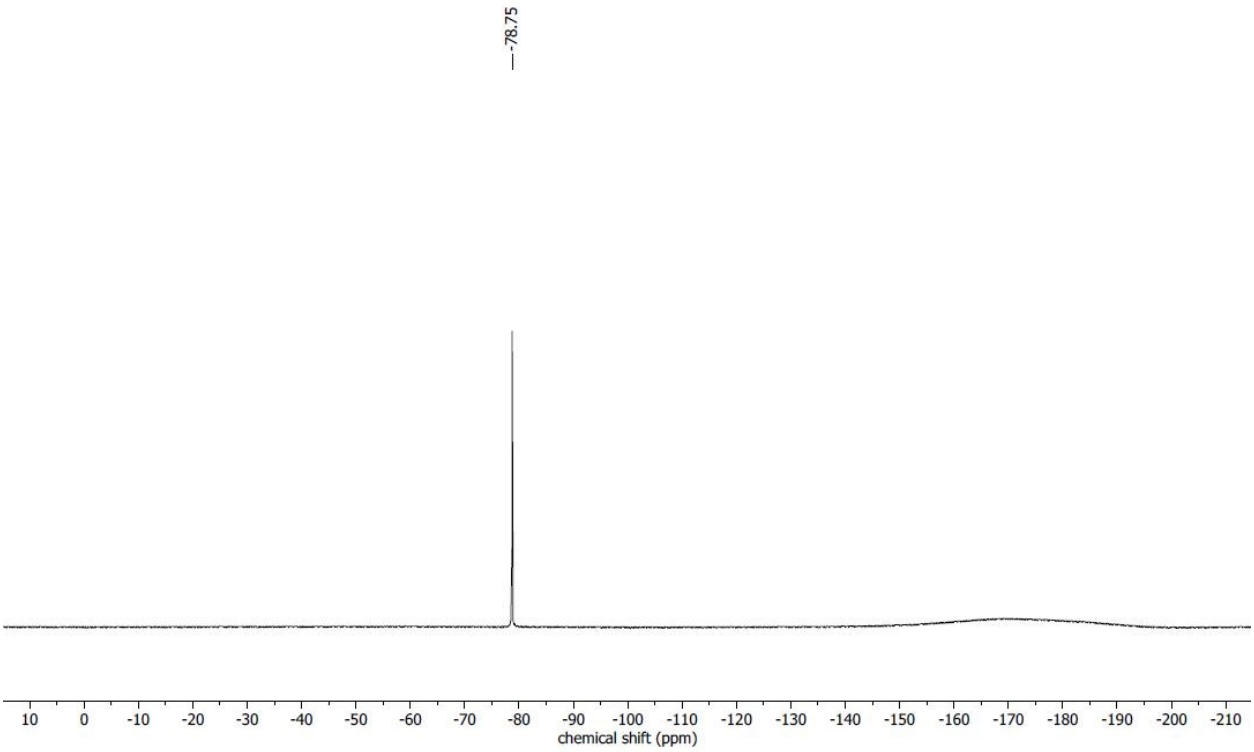


Figure S26: ^{19}F NMR spectrum of **4-Bi** in CD_2Cl_2.

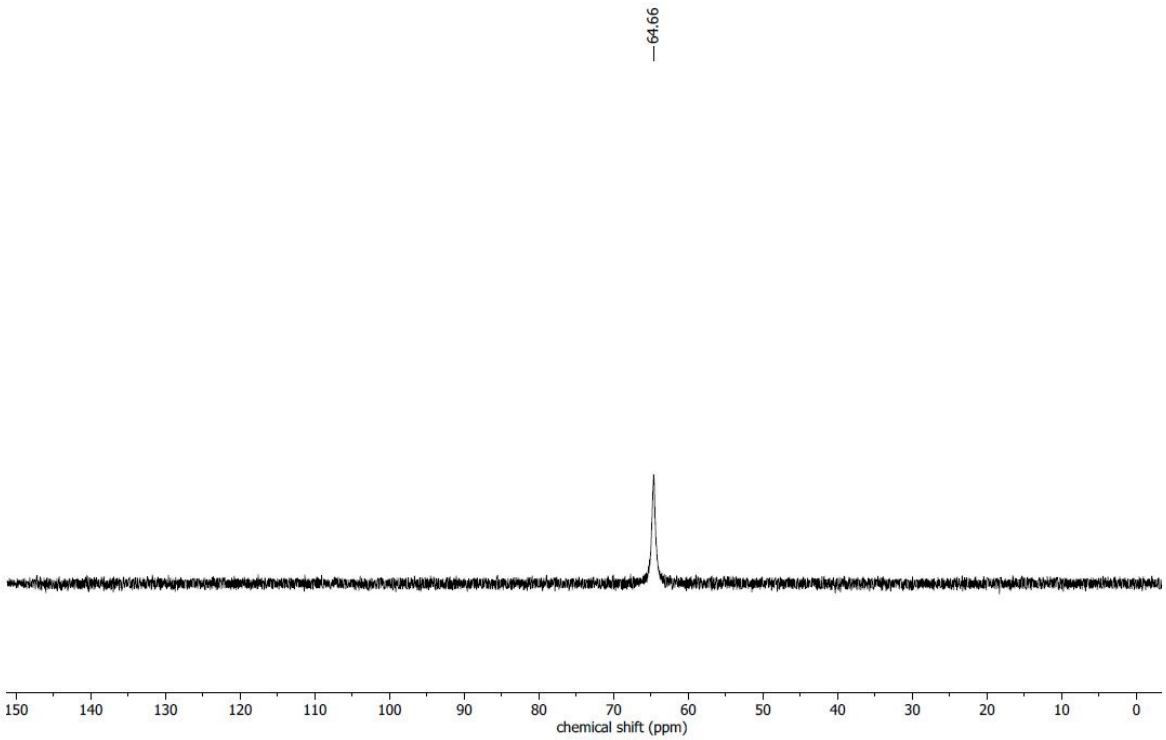


Figure S27: ^{31}P NMR spectrum of **4-Bi** in CD_2Cl_2.

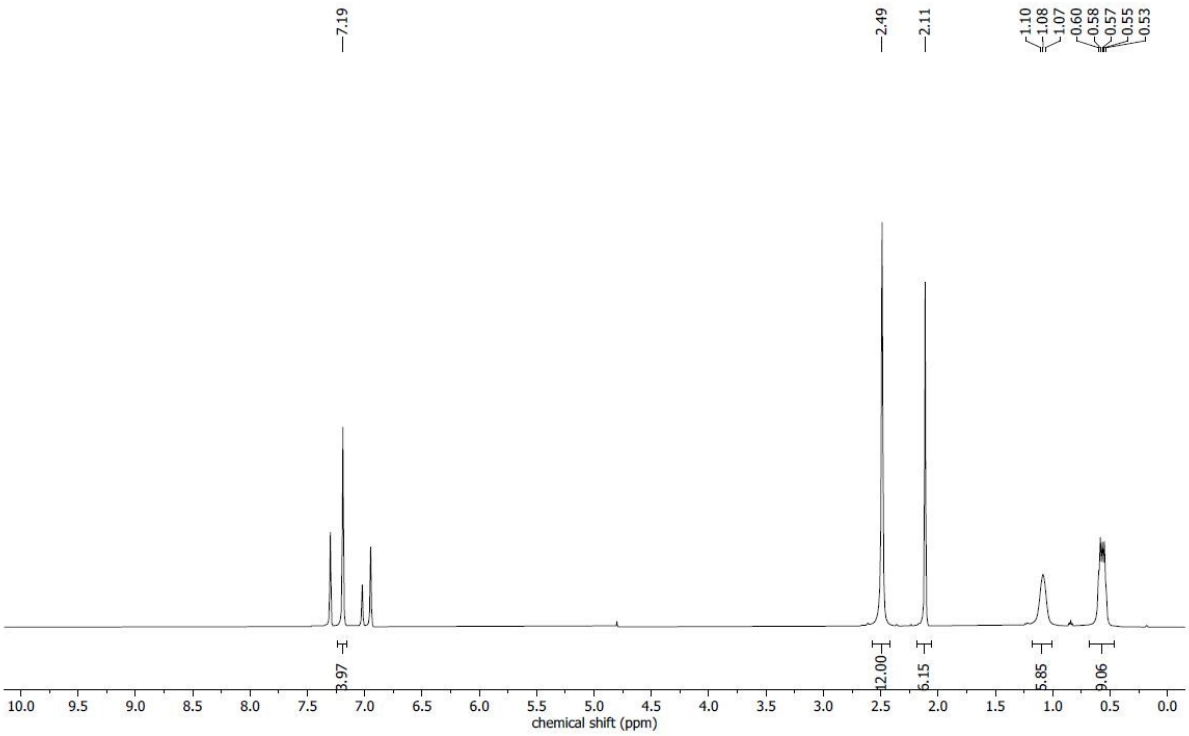


Figure S28: ^{1}H NMR spectrum of **4-Bi** in C_6D_5-Br.

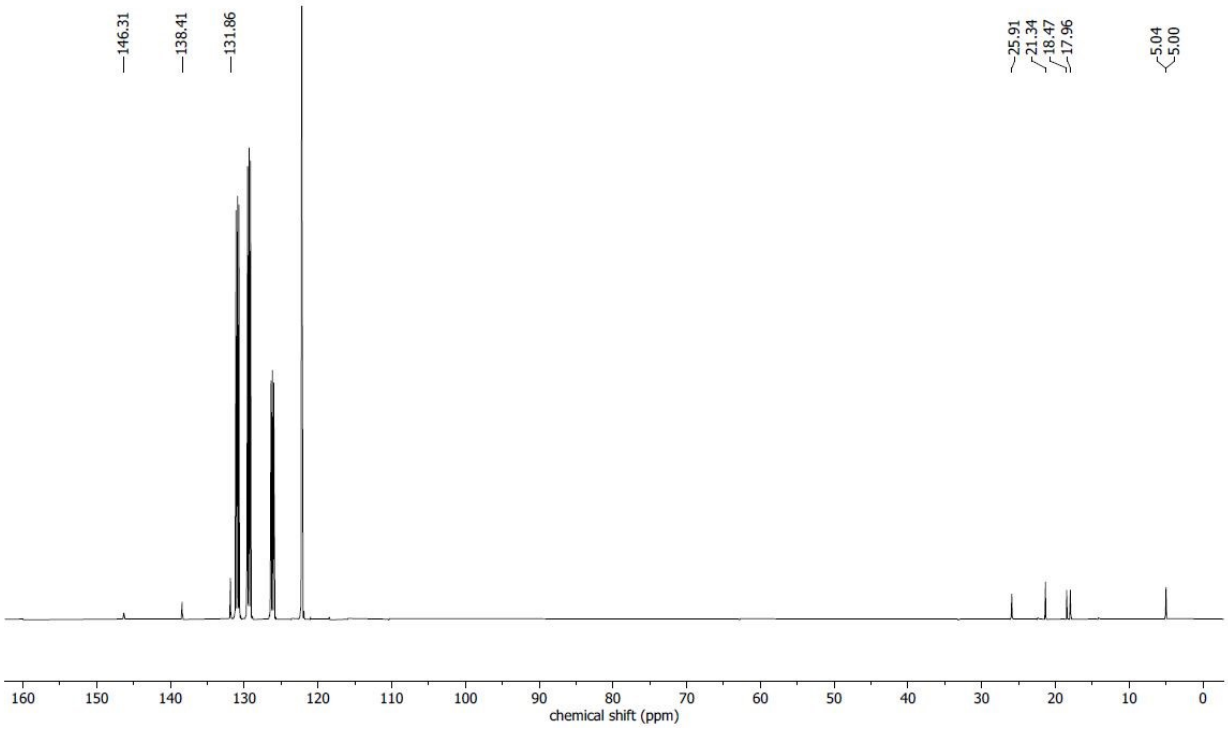


Figure S29: ^{13}C NMR spectrum of **4-Bi** in C_6D_5-Br.

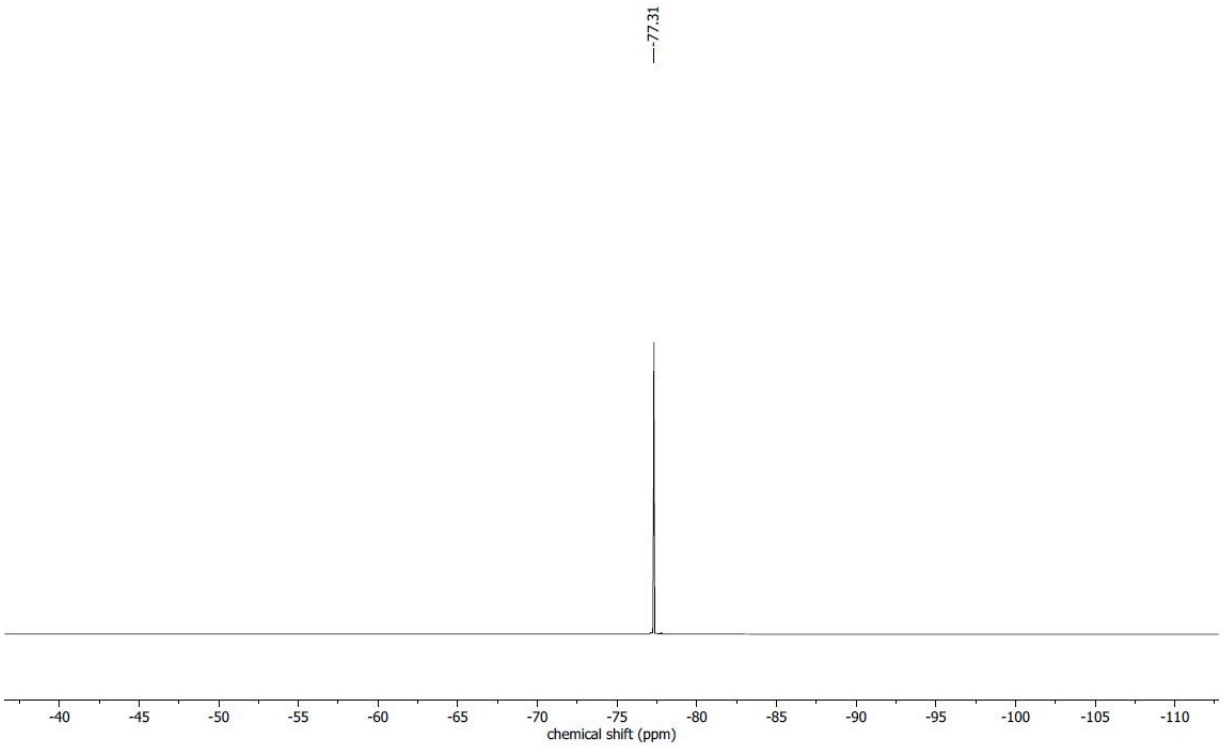


Figure S30: ^{19}F NMR spectrum of **4-Bi** in C_6D_5-Br.

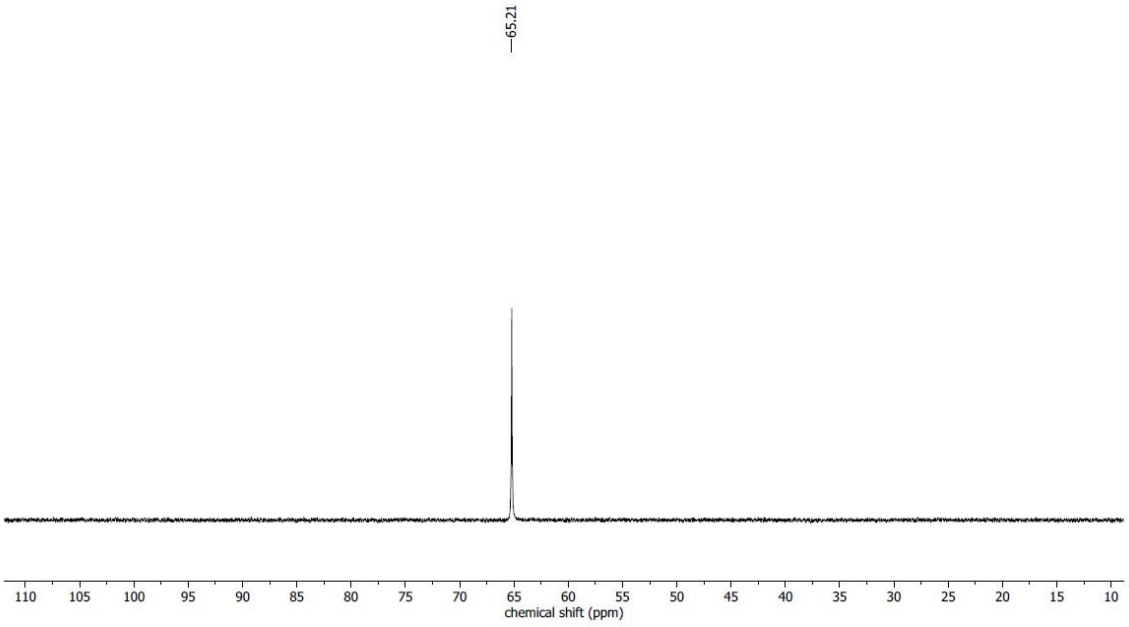


Figure S31: ^{31}P NMR spectrum of **4-Bi** in C_6D_5-Br.

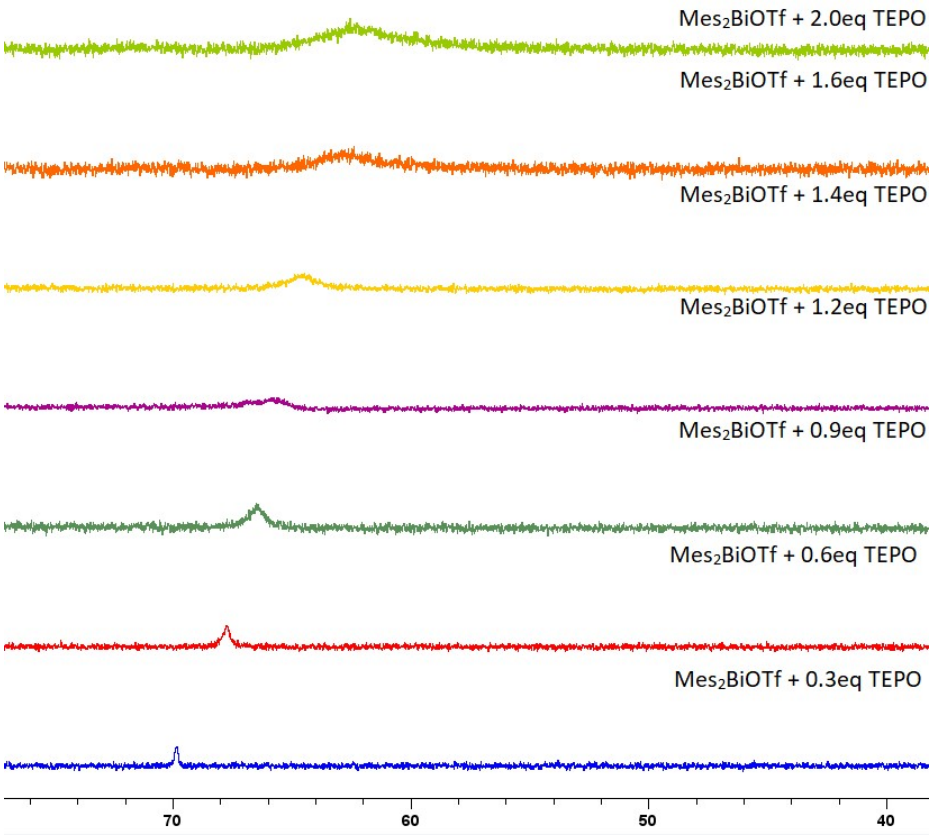


Figure S32: Stacked ^{31}P NMR spectrum of **3-Bi** in CD_2Cl_2 with varying concentration of Et_3PO.

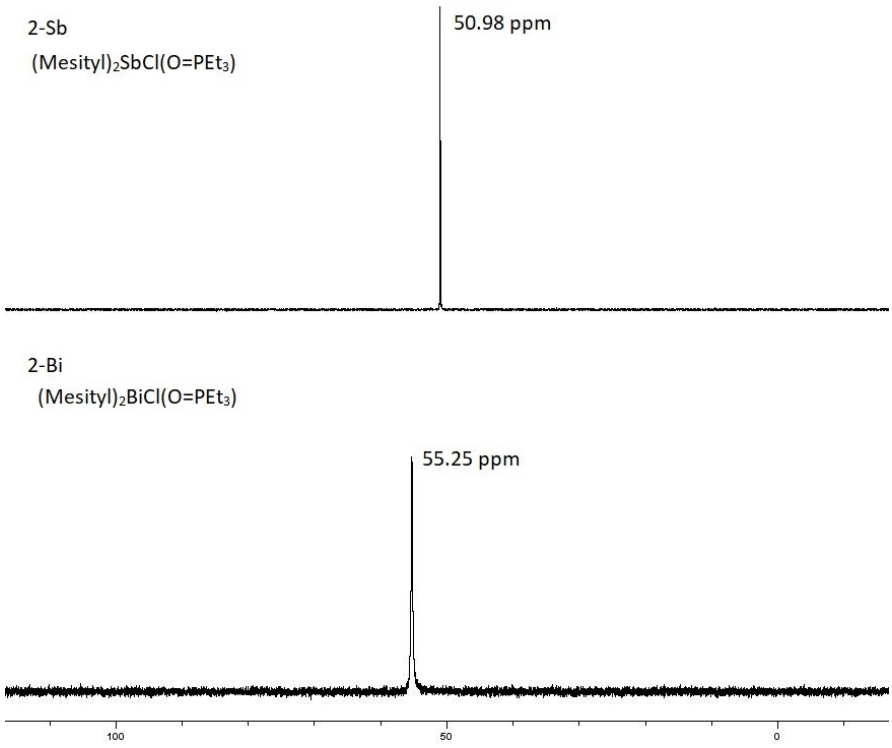


Figure S33: Stacked ^{31}P NMR spectrum of **2-Sb** vs **2-Bi.**

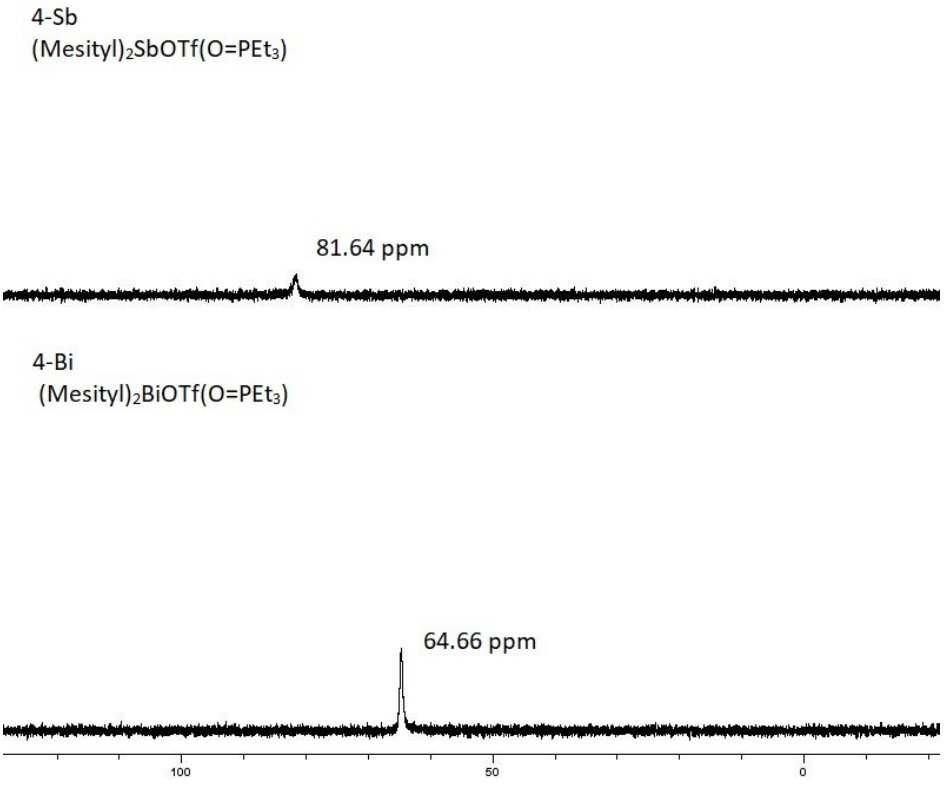


Figure S34: Stacked ^{31}P NMR spectrum of **4-Sb** vs **4-Bi.**

1.2 Catalysis

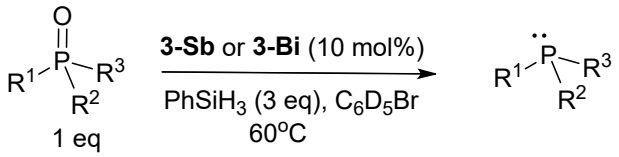
General method:

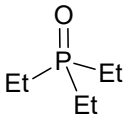
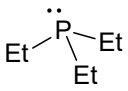
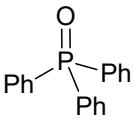
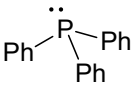
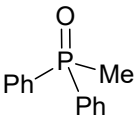
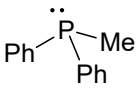
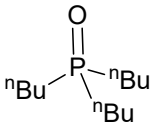
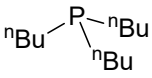
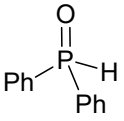
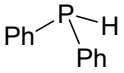
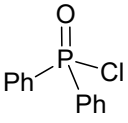
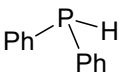
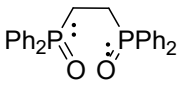
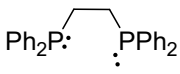
All the manipulations were carried out in argon atmosphere either using Schlenk techniques or glovebox. J Young NMR tubes were oven dried at 200 °C. The phosphine oxides were purchased from Sigma-Aldrich and used without any purification. The catalytic reactions were performed in C_6D_5-Br.

Experimental procedure for deoxygenation of phosphine oxide:

Catalyst, **3-Sb** (0.002 g, 0.0039 mmol) or **3-Bi** (0.002 g, 0.0033 mmol) and respective phosphine oxide (0.039 mmol for **3-Sb**, 0.033 mmol for **3-Bi**) were loaded into a J. Young NMR tube in glovebox. C_6D_5Br (0.6 mL) was added to the reaction mixture followed by 3 equivalents of $PhSiH_3$ (w.r.t. phosphine oxide). The NMR tube was then sealed, brought out of glovebox and transferred to an oil bath pre-heated at 60 °C. The reaction was then monitored at various time intervals by ^{1}H NMR and ^{31}P NMR until the conversion from phosphine oxide to phosphine was complete. NMR data is provided for the reaction mixture after the conversion.

Table S1. Reduction of phosphine oxides to respective phosphines catalyzed by **3-Sb** and **3-Bi**. Percentage of conversion was determined by ^{31}P NMR spectroscopy**.**



Substrate	Product	3-Sb		3-Bi	
		Time	conv(%)	Time	conv(%)
		24 hr	74	30 hr	66
		12 hr	92	30 hr	>97
		9 hr	>98	15 hr	>99
		29 hr	82	42 hr	71.5
		45 min	>99	1.25 hr	>99
		5 hr	>99	8.5 hr	>99
		36 hr	99	45 hr	66

NMR spectra for reduction of Phosphine oxides to phosphines:

<u>Triethylphosphine</u>

^{1}H NMR (500 MHz, C_6D_5Br): δ = 1.21 (m, 6H), 1.49 (m, 9H). ^{31}P NMR: δ = -19.4 ppm.

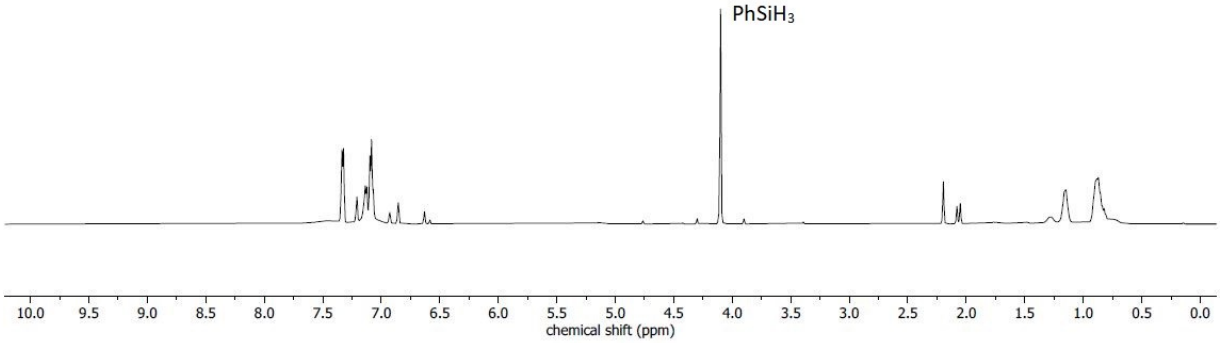


Figure S35: ^{1}H NMR spectrum in C_6D_5-Br.

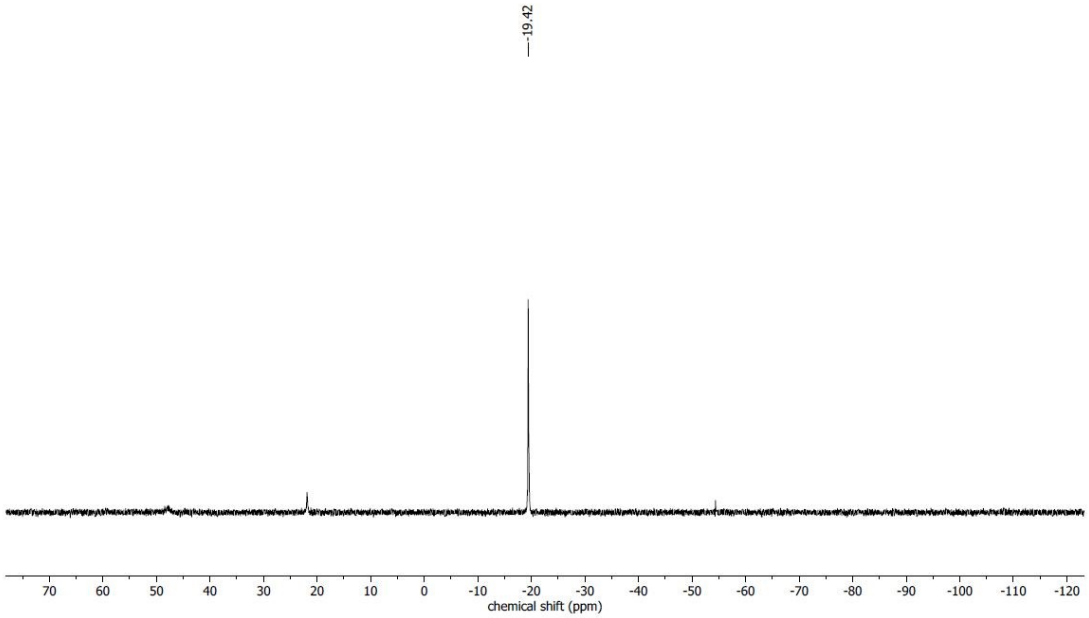


Figure S36: ^{31}P NMR spectrum in C_6D_5-Br.

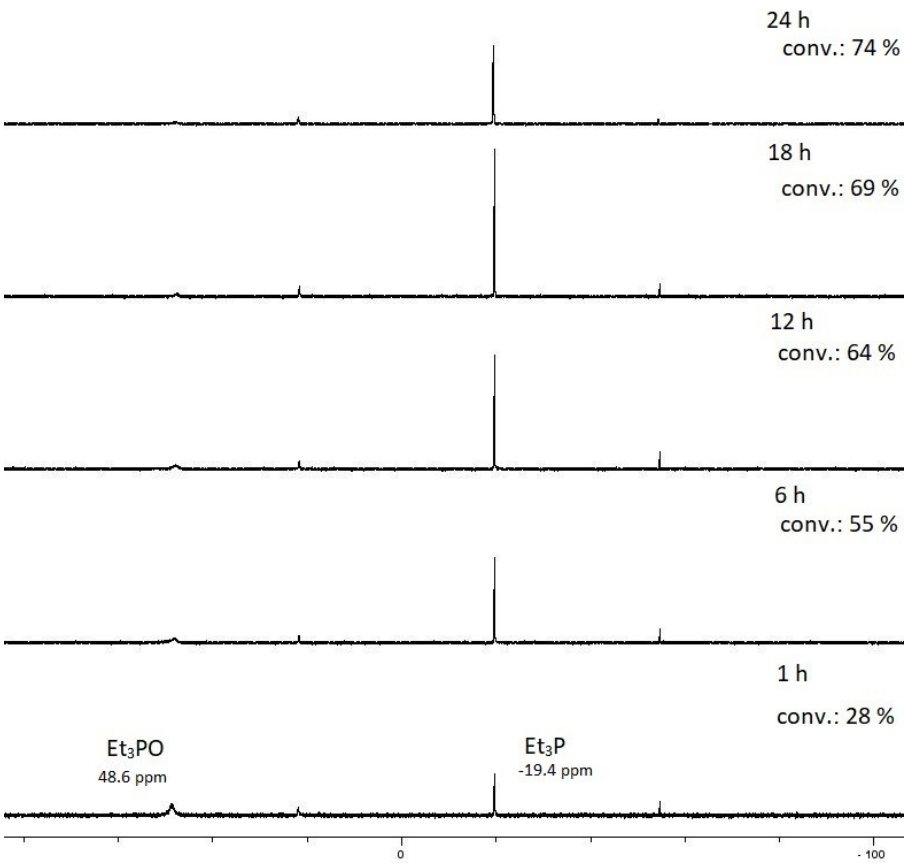


Figure S37: Stacked ^{31}P NMR spectrum of reduction of Et_3PO to Et_3P using catalyst **3-Sb** in C_6D_5-Br.

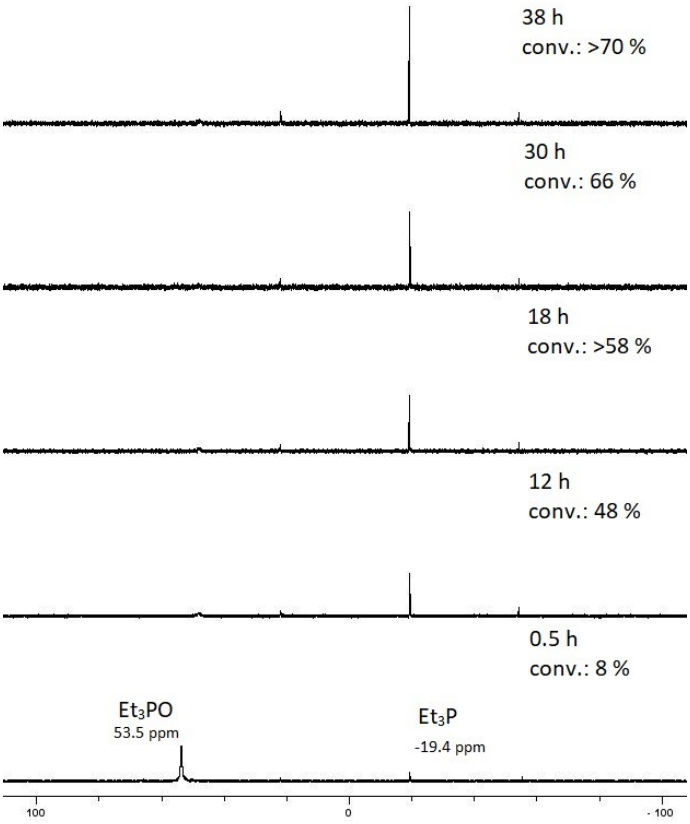


Figure S38: Stacked ^{31}P NMR spectrum of reduction of Et_3PO to Et_3P using catalyst **3-Bi** in C_6D_5-Br**.**

Triphenylphosphine

^{1}H NMR (500 MHz, C_6D_5Br): δ = 7.30 (6H), 7.20 (3H), 7.14 (6H) ppm. ^{31}P: δ = -5.5 ppm.

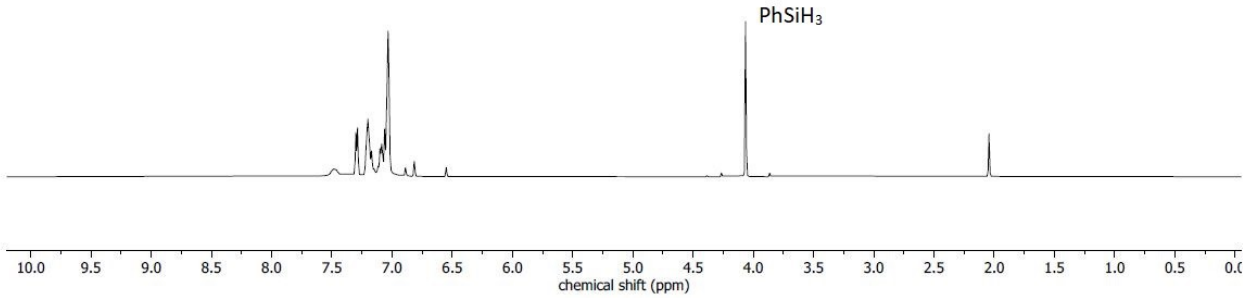


Figure S39: ^{1}H NMR spectrum in C_6D_5-Br.

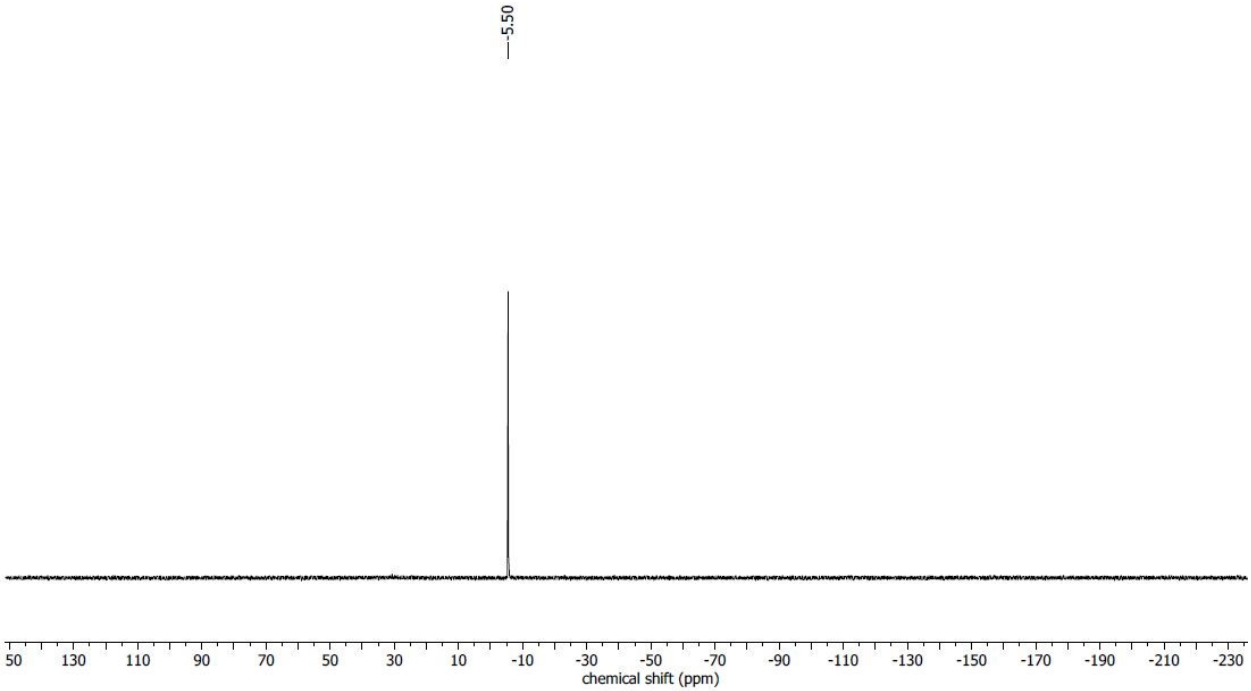


Figure S40: ^{31}P NMR spectrum in C_6D_5-Br.

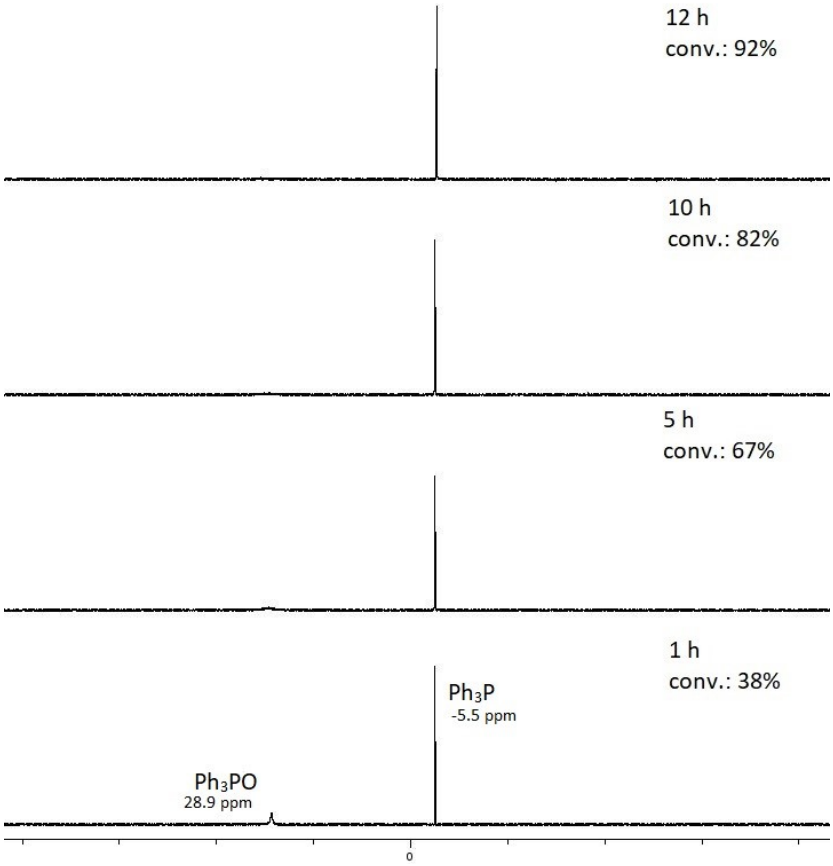


Figure S41: Stacked ^{31}P NMR spectrum of reduction of Ph_3PO to Ph_3P using catalyst **3-Sb** in C_6D_5-Br.

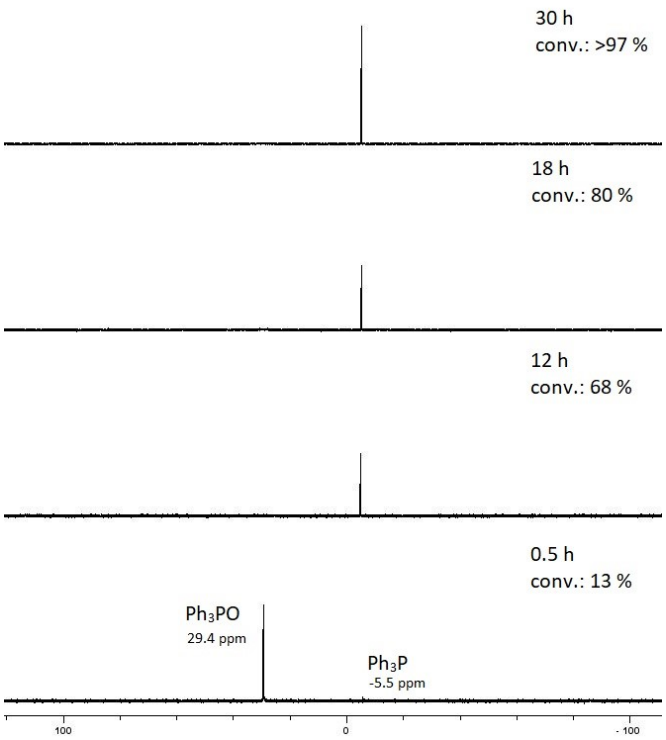


Figure S42: Stacked ^{31}P NMR spectrum of reduction of Ph_3PO to Ph_3P using catalyst **3-Bi** in C_6D_5-Br.

Methyldiphenylphosphine

^{1}H NMR (500 MHz, C_6D_5-Br): δ = 1.37 (s, br, 3H), 7.04–7.07 (m, 7H), 7.36 (m, 3H).

^{31}P NMR: δ = -26.7 ppm.

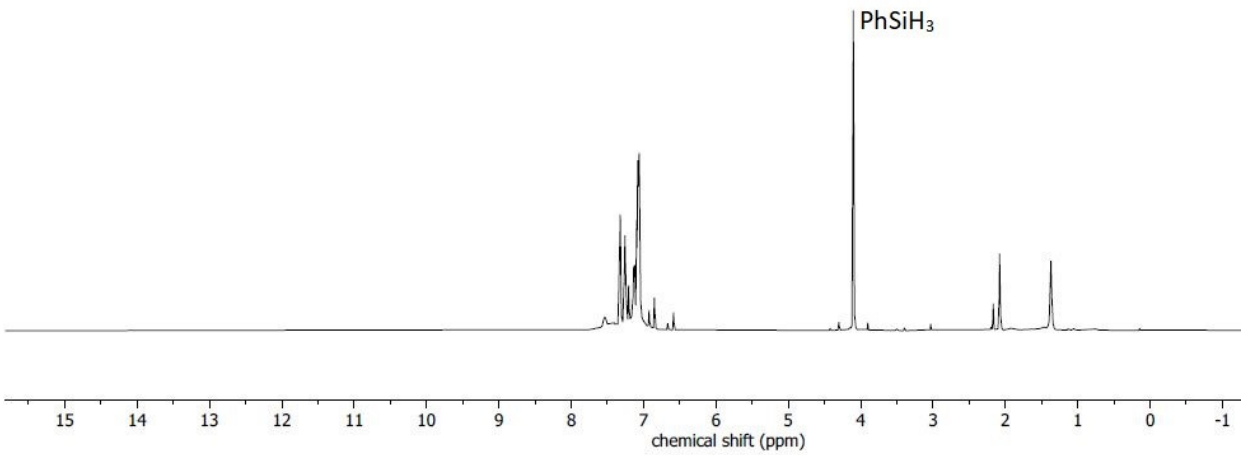


Figure S43: ^{1}H NMR spectrum in C_6D_5-Br.

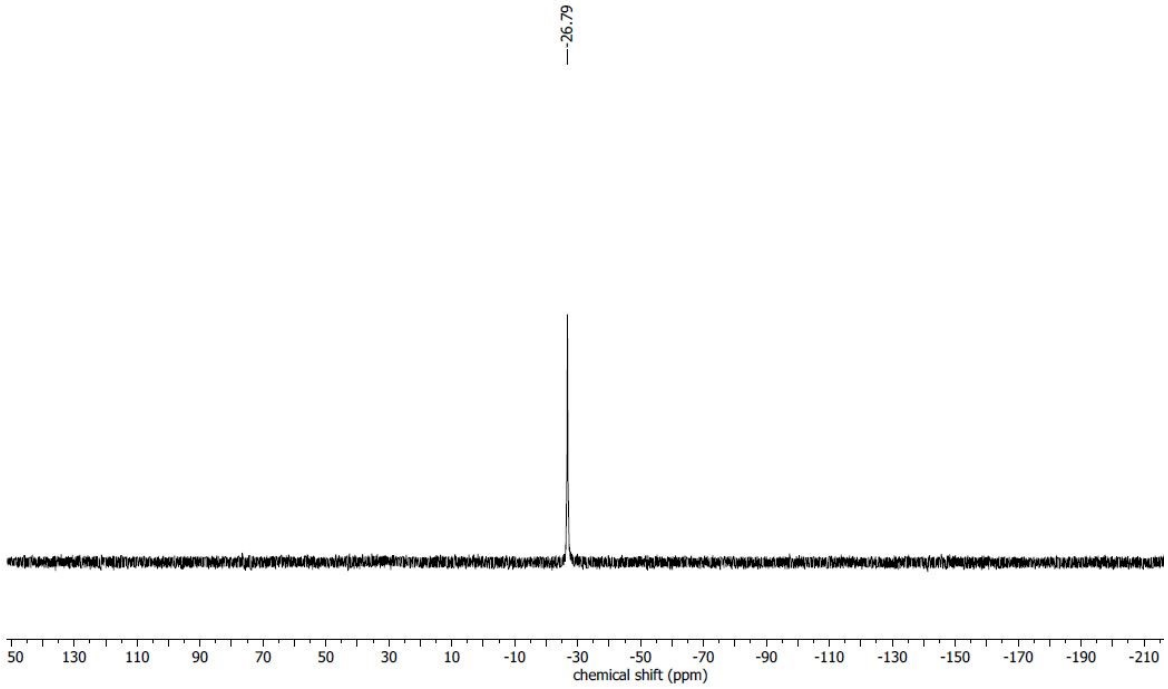


Figure S44: ^{31}P NMR spectrum in C_6D_5-Br.

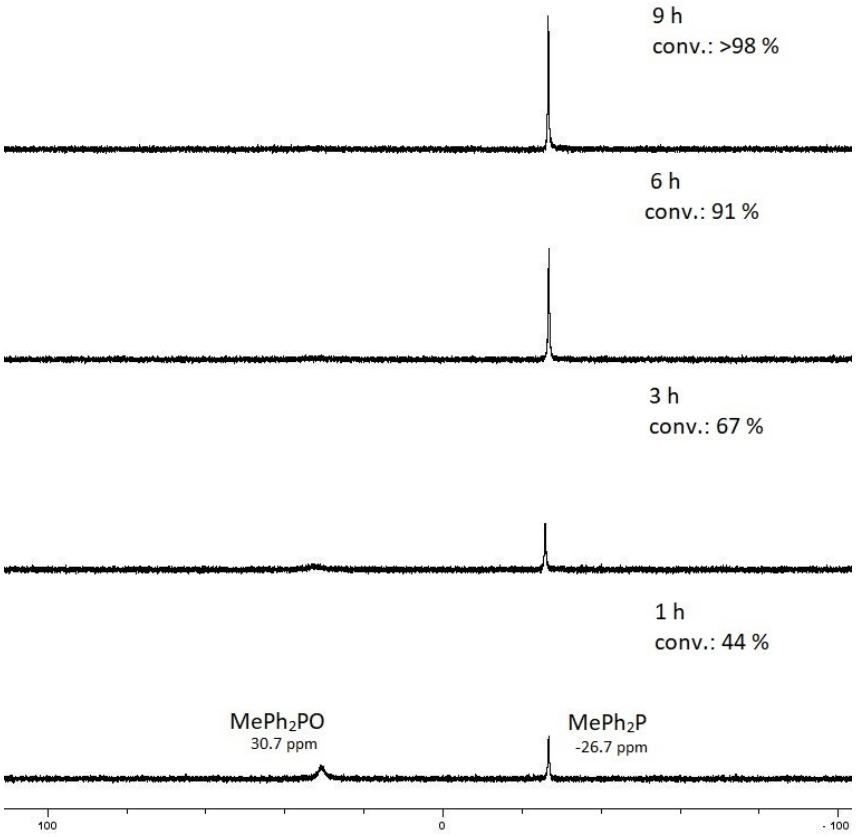


Figure S45: Stacked ^{31}P NMR spectrum of reduction of $MePh_2PO$ to $MePh_2P$ using catalyst **3-Sb** in C_6D_5- Br.

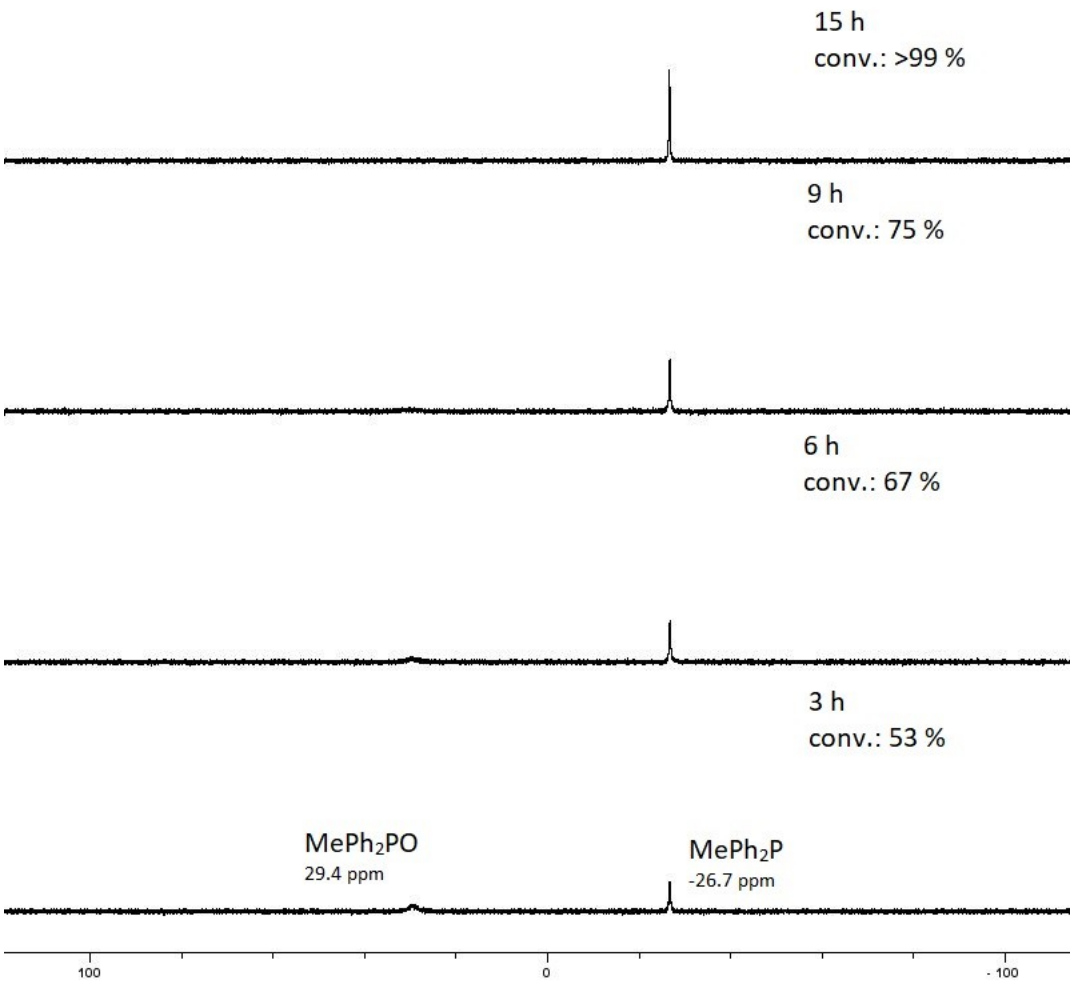


Figure S46: Stacked ^{31}P NMR spectrum of reduction of $MePh_2PO$ to $MePh_2P$ using catalyst **3-Bi** in C_6D_5-Br.

Diphenylphosphine

^{1}H NMR (500 MHz, C_6D_5-Br): δ = 5.20 (d, J = 216.3 Hz, 1H), 7.11-7.16 (br, 6H), 7.37-7.42 (br, 4H)

^{31}P NMR: δ = -39.9 ppm.

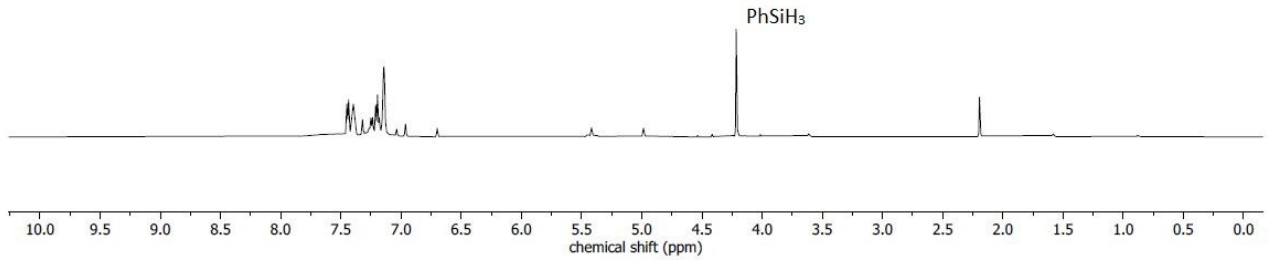


Figure S47: ^{1}H NMR spectrum in C_6D_5-Br.

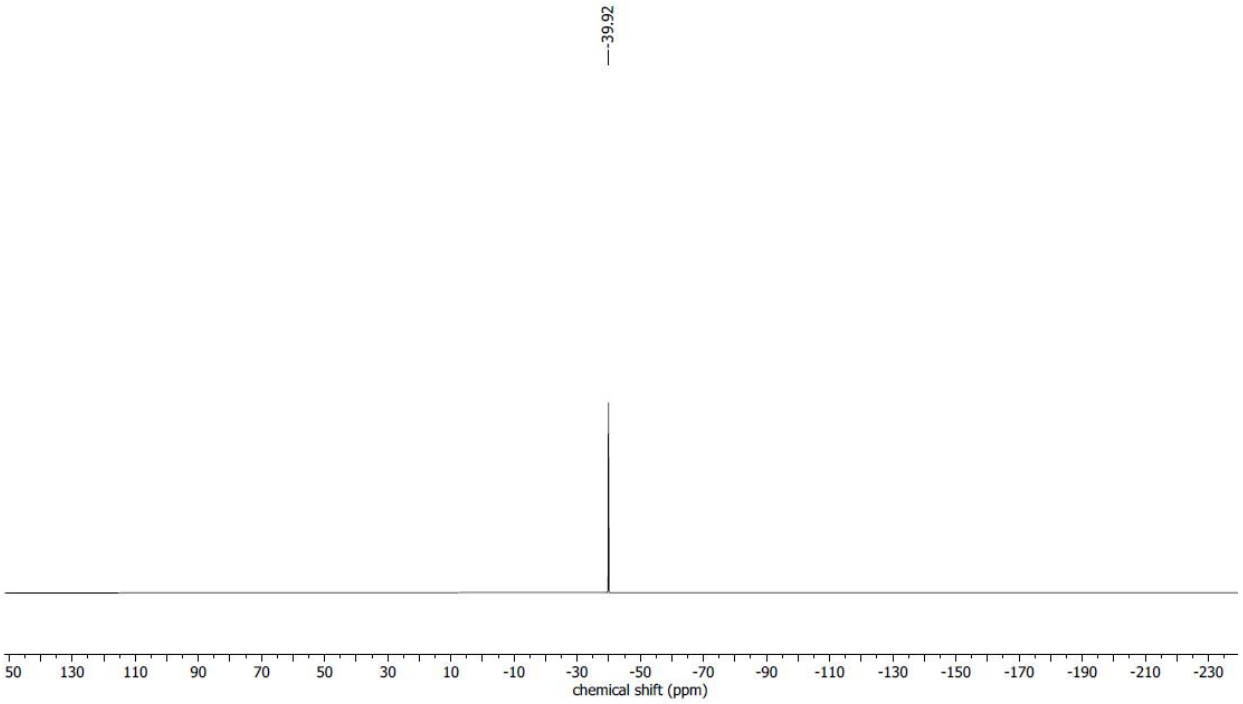


Figure S48: ^{31}P NMR spectrum in C_6D_5-Br.

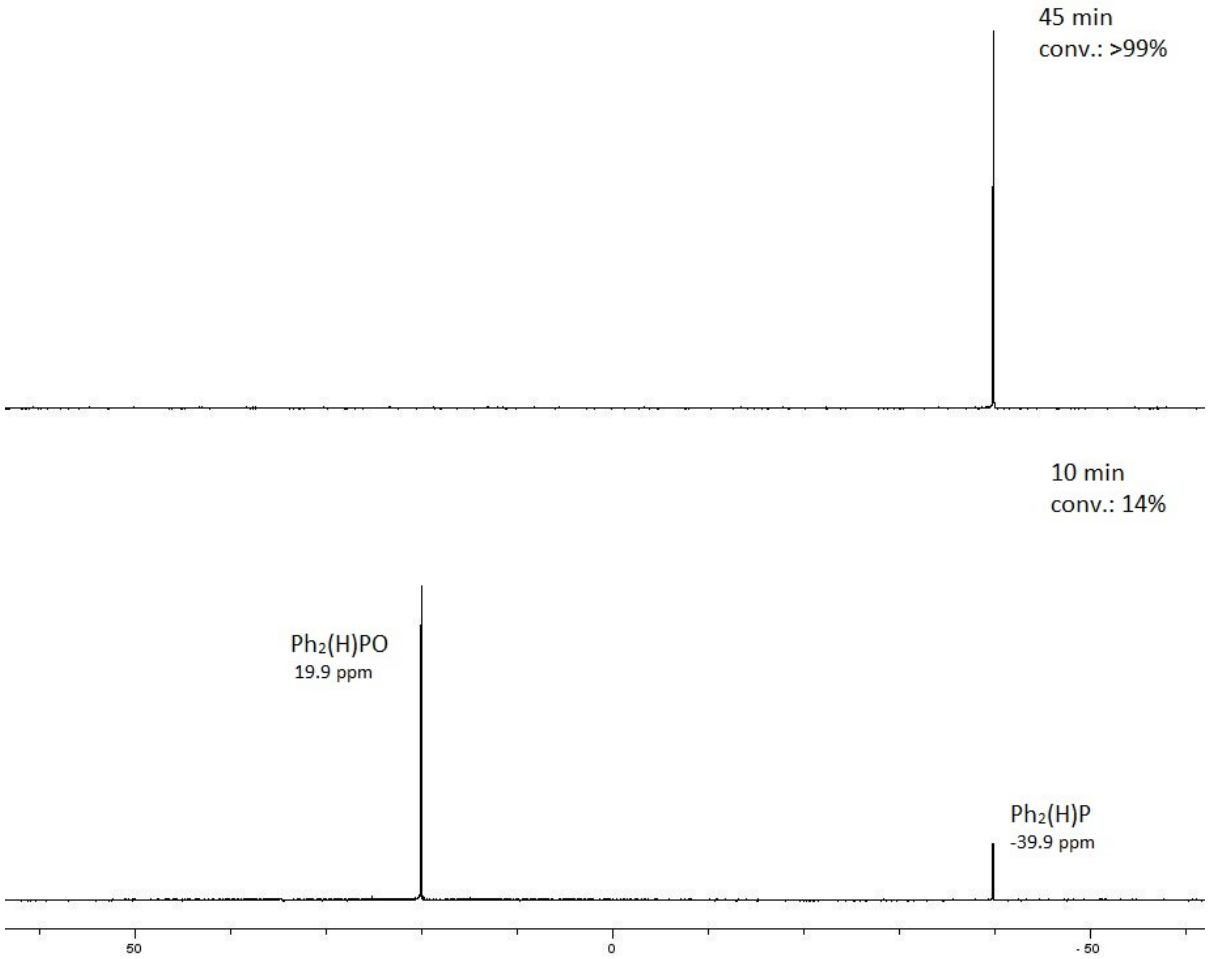


Figure S49: Stacked ^{31}P NMR spectrum of reduction of $Ph_2(H)PO$ to Ph_2PH using catalyst **3-Sb** in C_6D_5- Br.

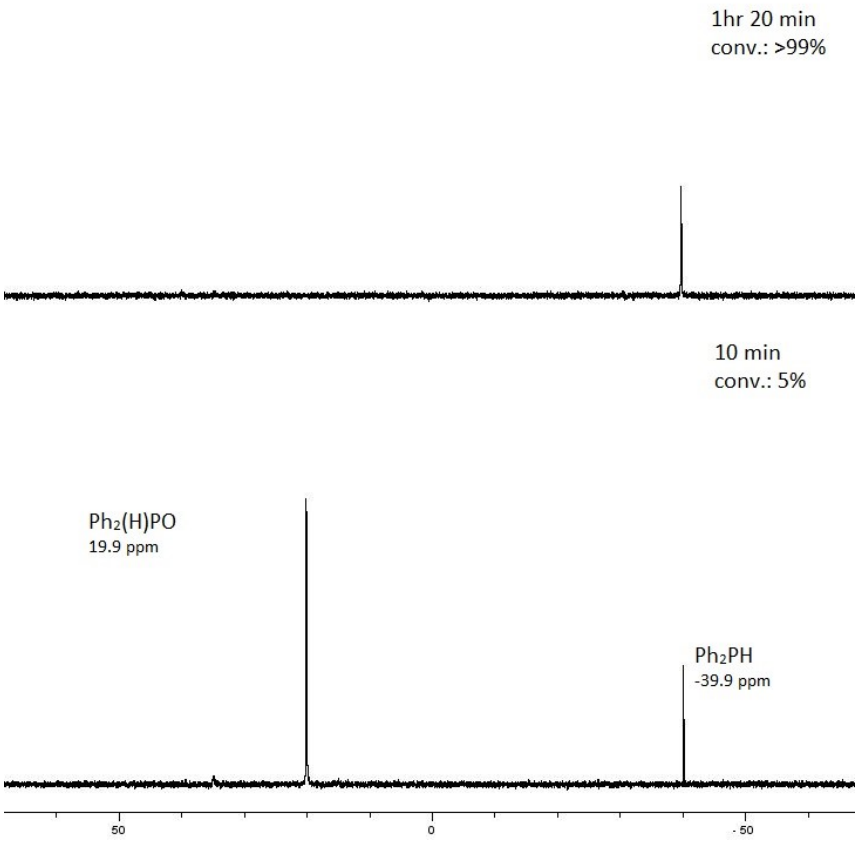


Figure S50: Stacked ^{31}P NMR spectrum of reduction of $Ph_2(H)PO$ to Ph_2PH using catalyst **3-Bi** in C_6D_5- Br.

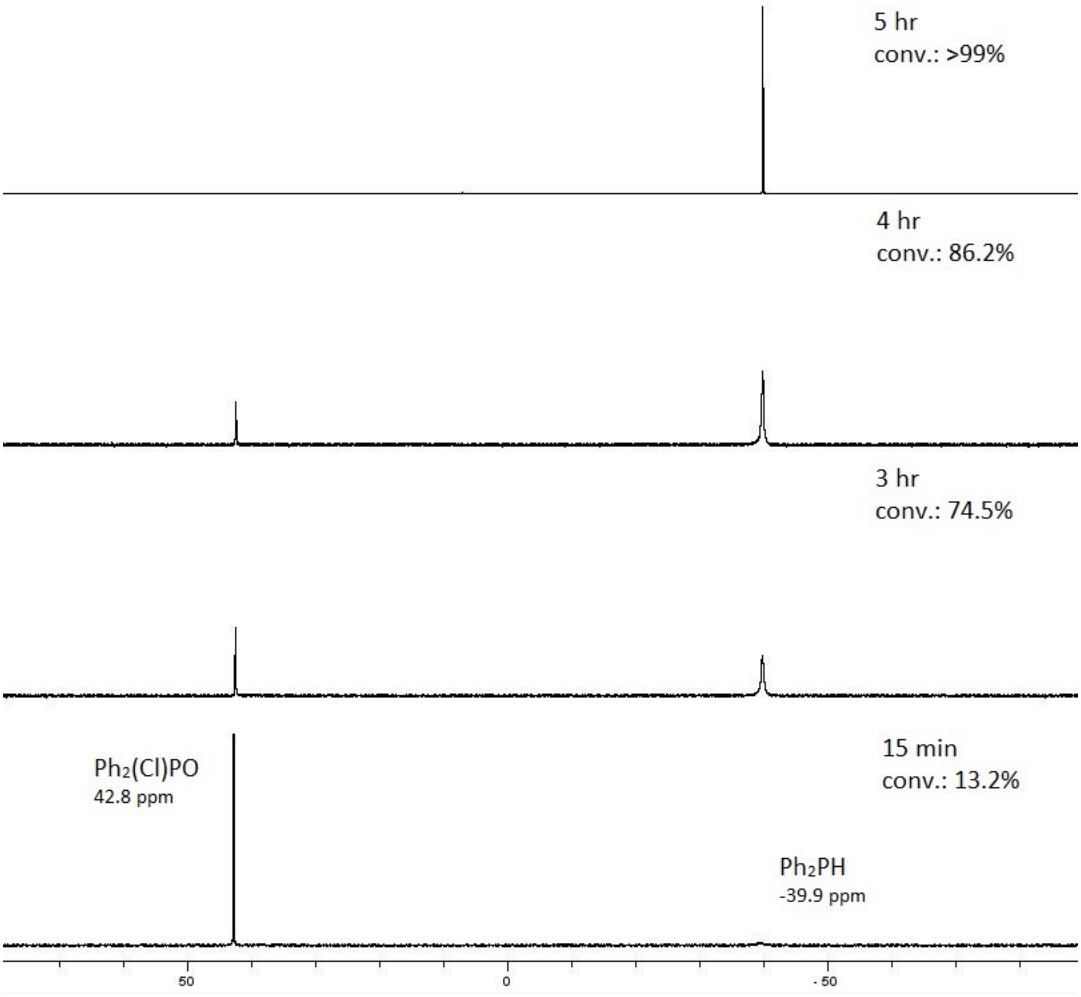


Figure S51: Stacked ^{31}P NMR spectrum of reduction of $Ph_2(Cl)PO$ to Ph_2PH using catalyst **3-Sb** in C_6D_5- Br.

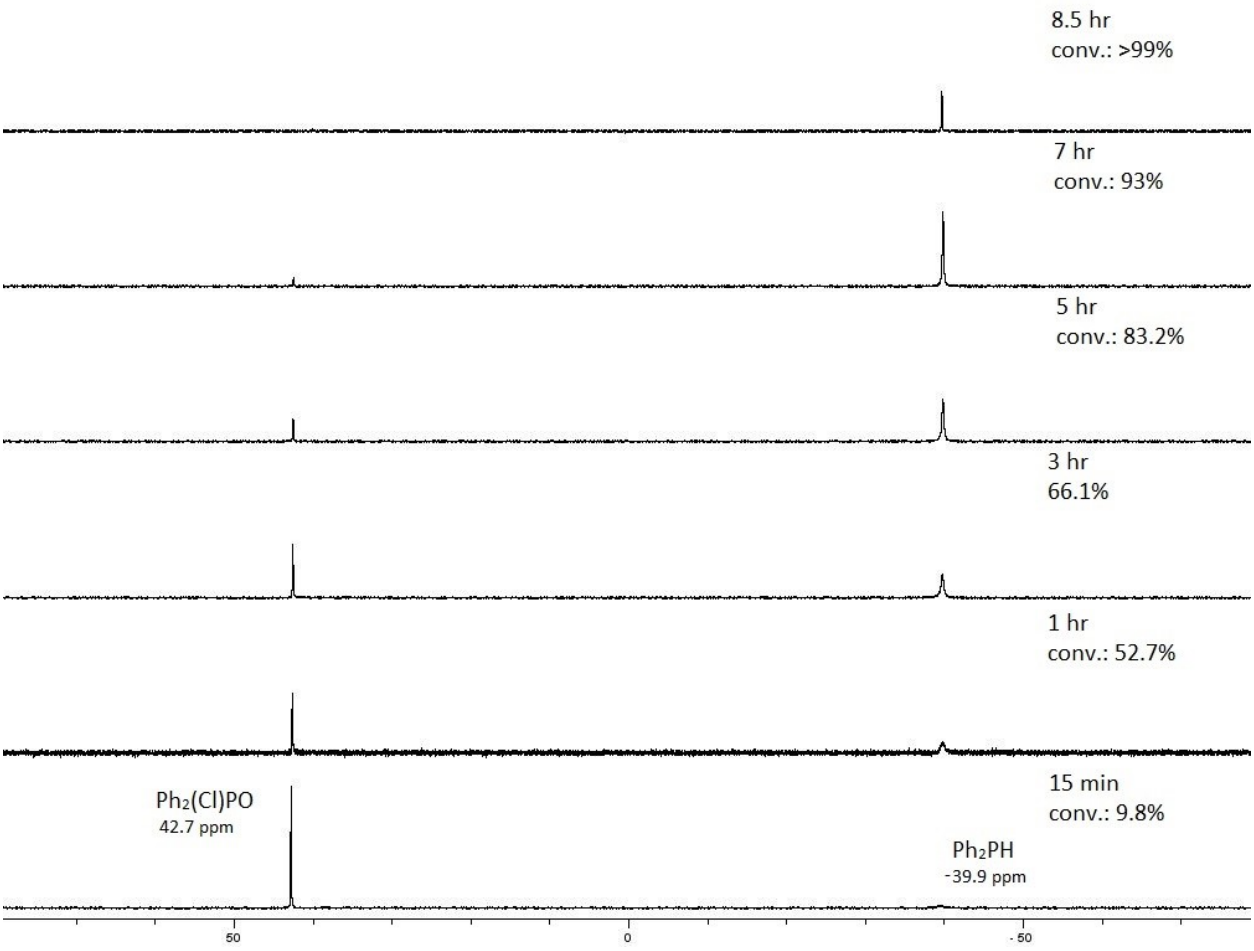


Figure S52*:* Stacked ^{31}P NMR spectrum of reduction of $Ph_2(Cl)PO$ to Ph_2PH using catalyst **3-Bi** in C6D5- Br.

<u>1,2-Bis(diphenylphosphino)ethane</u>

^{1}H NMR (500 MHz, C_6D_5-Br): δ = 01.10(d,2H), 1.58(d,2H), 7.11-7.16 (br, 6H), 7.37-7.42 (br, 4H)

^{31}P NMR: δ = -12.5 ppm.

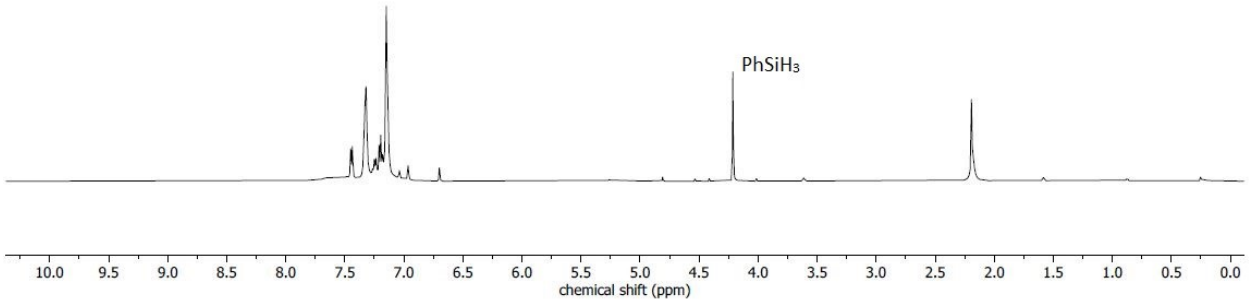


Figure S53: ^{1}H NMR spectrum in C_6D_5-Br.

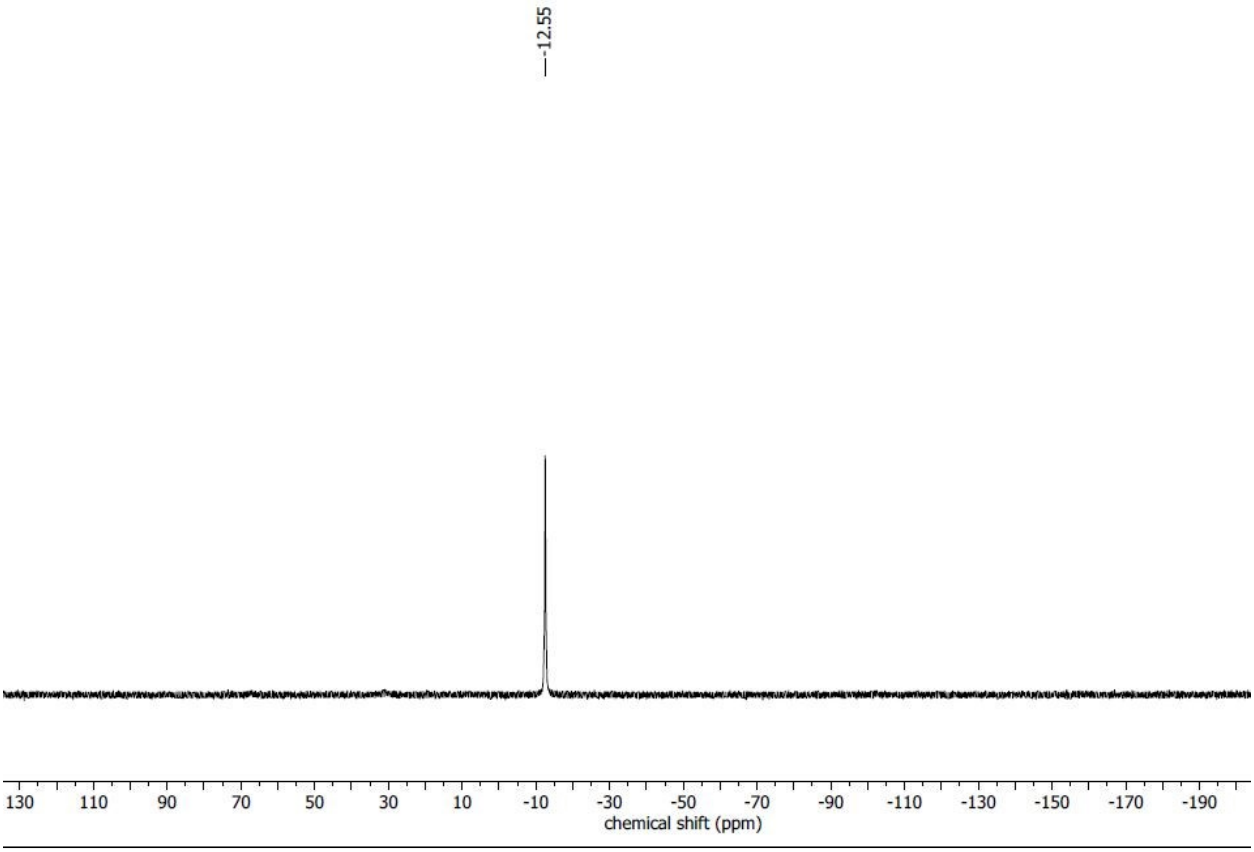


Figure S54: ^{31}P NMR spectrum in C_6D_5-Br.

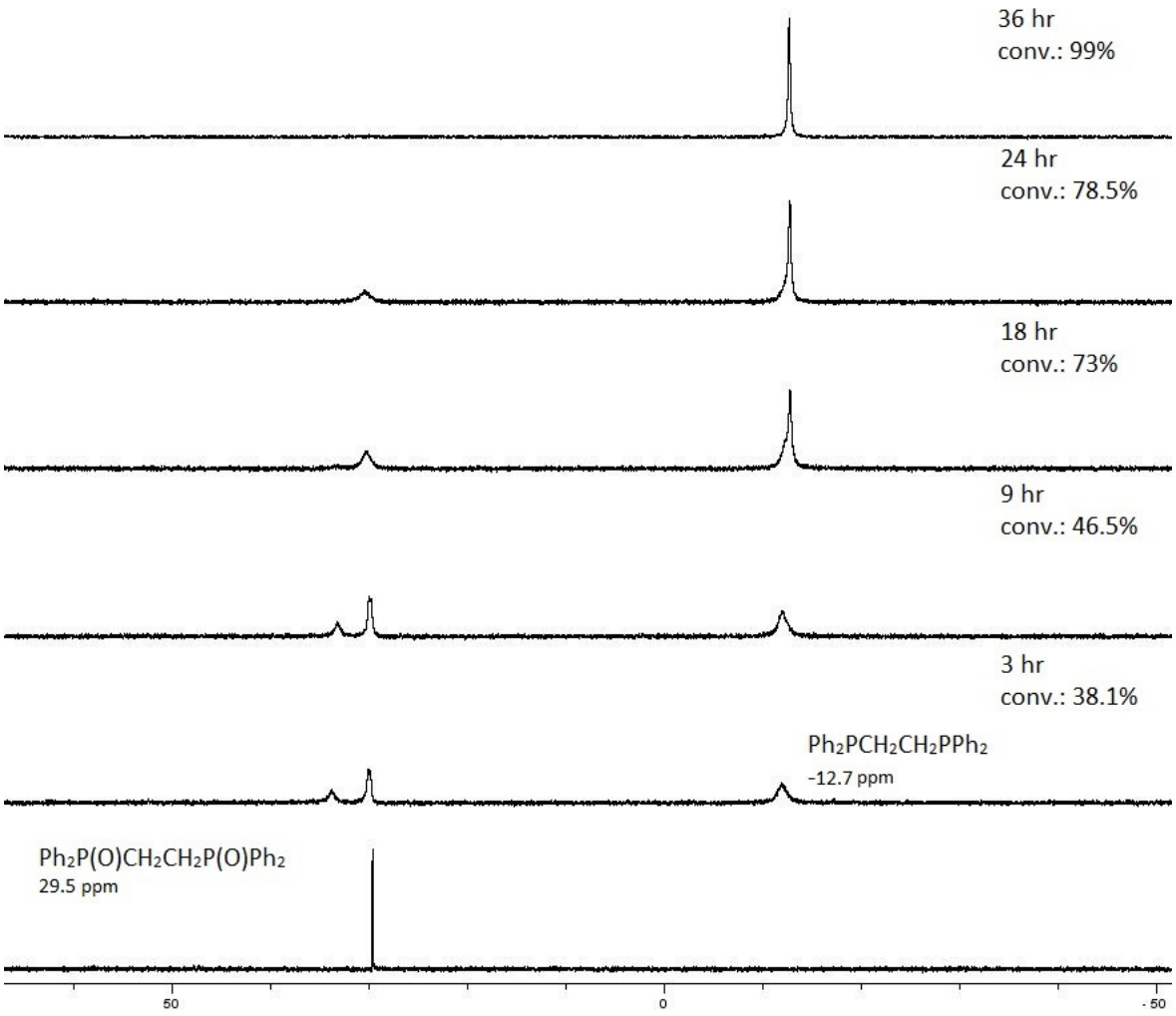


Figure S55*:* Stacked ^{31}P NMR spectrum of reduction of $Ph_2(O)P(CH_2)_2P(O)Ph_2$ to $Ph_2P(CH_2)_2PPh_2$ using catalyst **3-Sb** in C_6D_5- Br.

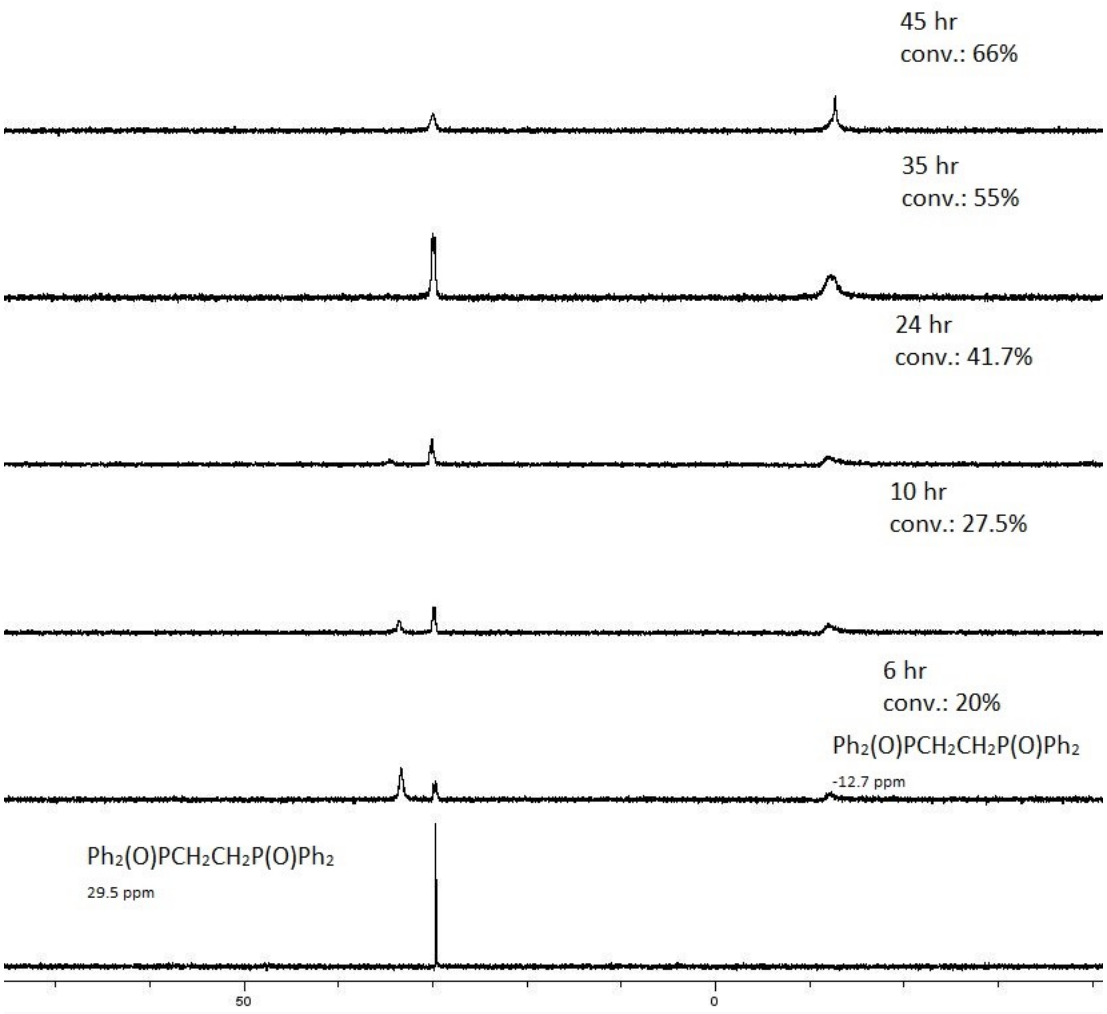


Figure S56: Stacked ^{31}P NMR spectrum of reduction of $Ph_2(O)P(CH_2)_2P(O)Ph_2$ to $Ph_2P(CH_2)_2PPh_2$ using catalyst **3-Bi** in C_6D_5- Br.

<u>Tributylphosphine</u>

^{1}H NMR (500 MHz, C_6D_5-Br): δ = 0.9(m,9H), 1.39(m,18H)

^{31}P NMR: δ = -31.6 ppm.

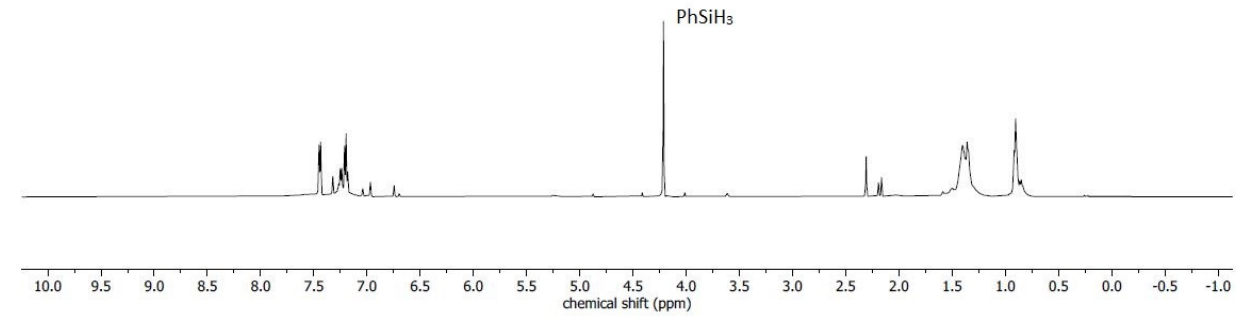


Figure S57: : ^{1}H NMR spectrum in C_6D_5-Br.

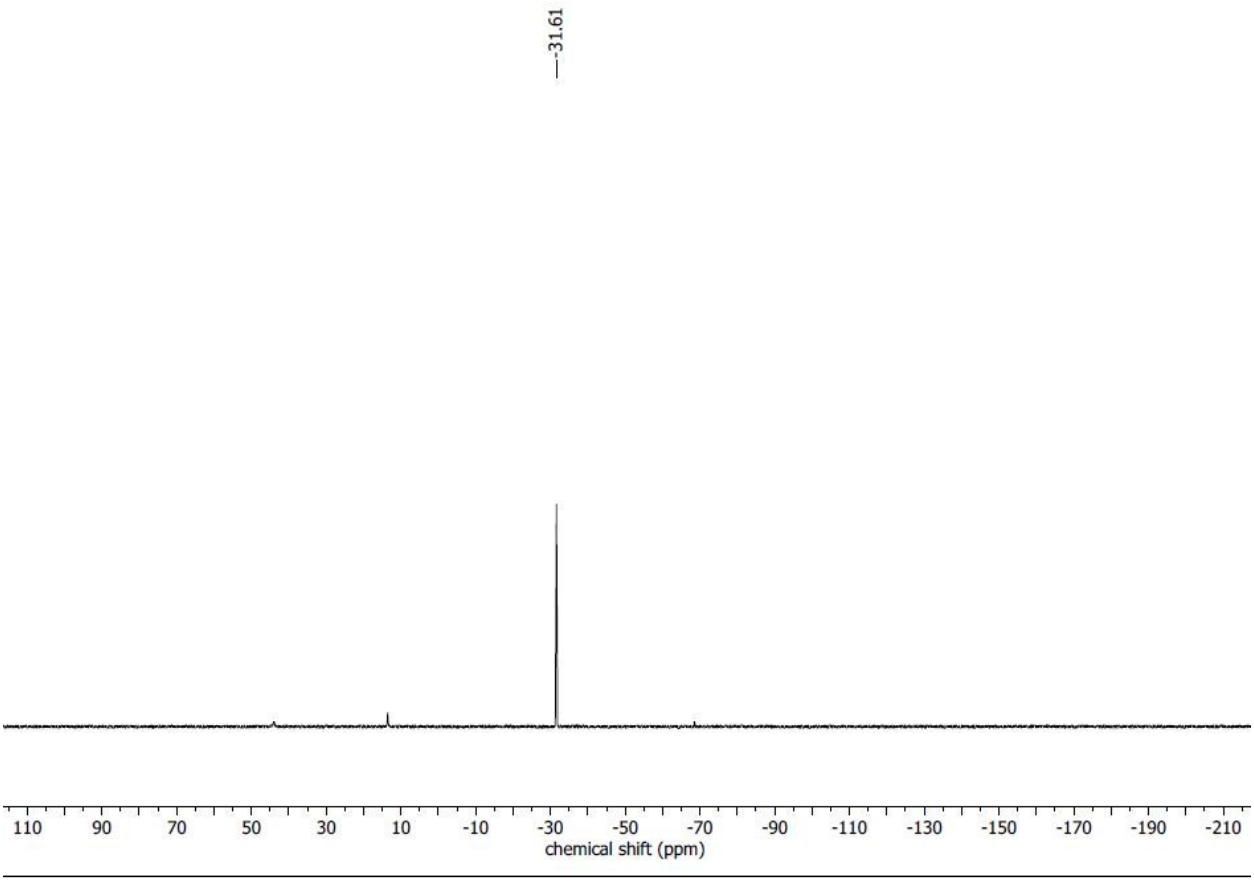


Figure S58: : ^{31}P NMR spectrum in C_6D_5-Br.

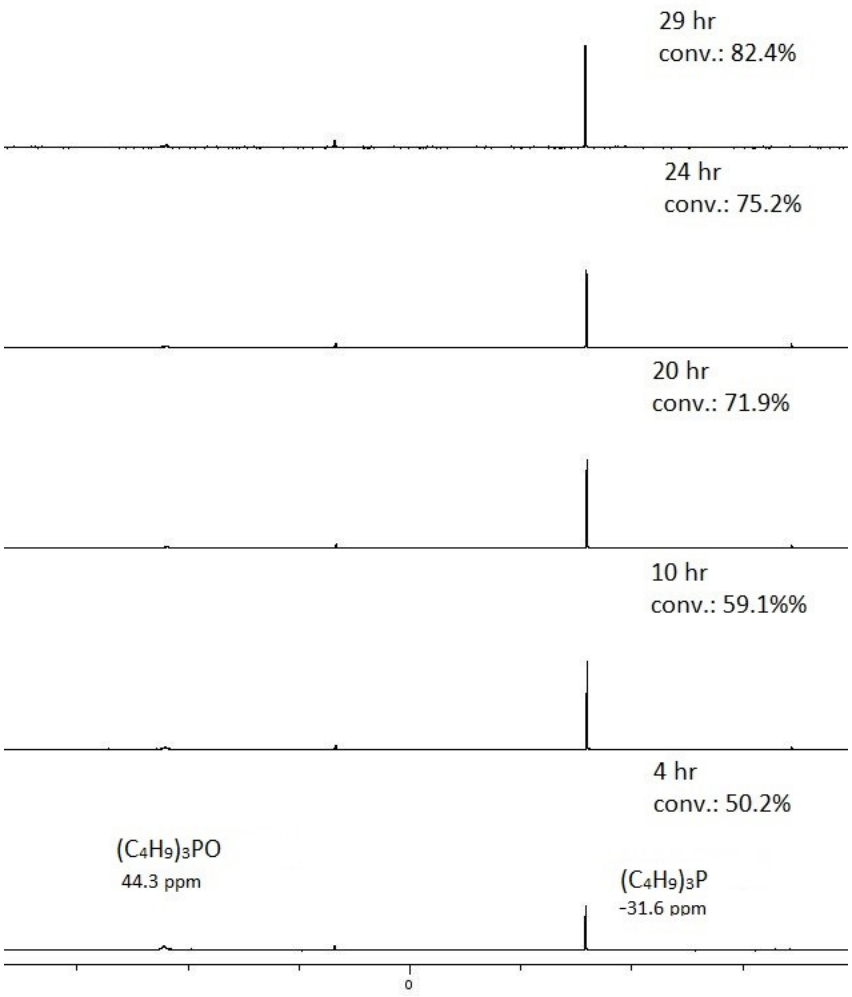


Figure S59: Stacked ^{31}P NMR spectrum of reduction of $(C_4H_9)_3PO$ to $(C_4H_9)_3P$ using catalyst **3-Sb** in C_6D_5- Br.

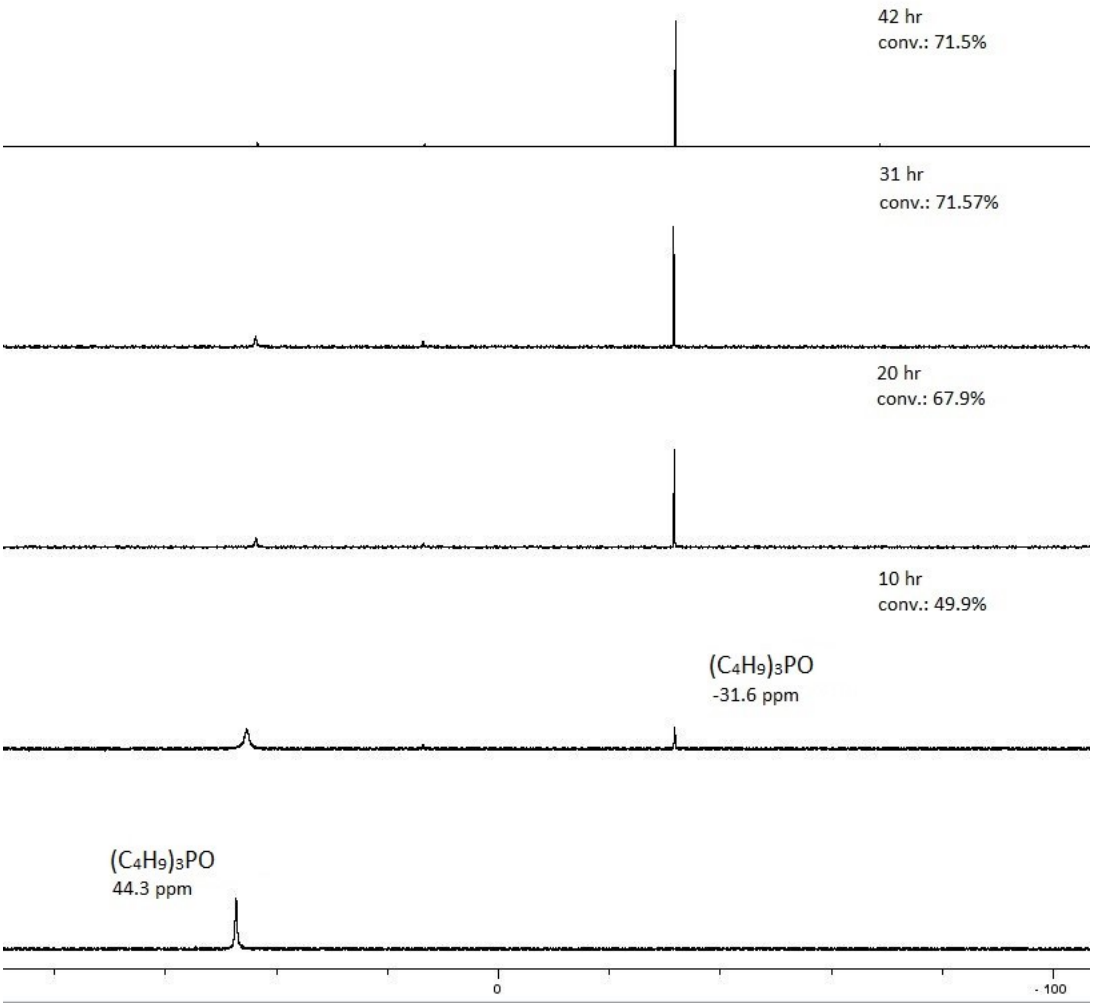


Figure S60: Stacked ^{31}P NMR spectrum of reduction of $(C_4H_9)_3PO$ to $(C_4H_9)_3P$ using catalyst **3-Bi** in C_6D_5- Br.

2. Crystallographic Data

Crystals were layered with Paratone oil before mounting on diffractometer. Single-crystal X-ray crystallography for structural analysis was performed on a Bruker Kappa APEX II CCD Diffractometer, using Mo-Kα radiation, having a wavelength of 0.71073 Å, equipped with a CCD detector by using the APEX software package.[6] A matrix scan was used to determine the initial lattice parameters. Reflections were merged and corrected for Lorenz and polarization effects and background using SAINT.[7] Absorption corrections, including odd and even ordered spherical harmonics were performed using SADABS.[8] Space group assignments were based upon systematic absences, E statistics, and successful refinement of the structures. The structures were solved by SHELXT (version 2018/2) and refined by SHELXTL (version 2018/3) software package installed in the platform WinGX.[9,10] All non-hydrogen atoms, including those in disordered molecules, were refined anisotropically. Hydrogen atoms are placed at calculated positions and refined using a riding model.

In **4-Sb**, the solvent used for crystallization was dichloromethane and layered with pentane. Final Fourier difference electron density map showed the presence of pentane in the lattice. However, the solvent molecule was so entangled by disorder that it was not possible to model them to chemically meaningful positions. Hence the solvent molecule was squeezed. In both **4-Sb** and **4-Bi** the portion of the 'triethyl-phosphine oxide ($O=PEt_3$)" was found to be disordered and was modelled with two orientations with relative occupancies of 0.68:0.32 and 0.65:0.35 respectively for the two parts.

Table S2. Crystal data and structure refinement for **3-Sb.**

Identification code	3-Sb	
CCDC Number	2086626	
Empirical formula	$C_{19}H_{22}F_3O_3SSb$	
Formula weight	509.17	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	*P*-1	
Unit cell dimensions	*a* = 7.2653(19) Å	*α* = 85.443(8)°
	b = 16.097(4) Å	*β* = 89.167(9)°
	c = 17.027(5) Å	*γ* = 84.022(8)°
Volume	1974.2(9) $Å^3$	
Z	4	
Density (calculated)	1.713 mg/m^3	
Absorption coefficient	1.547 mm^{-1}	
F(000)	1016	
Crystal size	0.058 x 0.047 x 0.035 mm^3	
Theta range for data collection	1.200 to 24.999°	
Index ranges	-8<=h<=8, -19<=k<=19, -20<=l<=20	
Reflections collected	43116	
Independent reflections	6962 [R_{int} = 0.0774]	
Completeness to theta = 24.999°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.948 and 0.916	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6962 / 6 / 492	
Goodness-of-fit on F^2	1.112	
Final R indices [I>2sigma(I)]	R_1 = 0.0642, wR_2 = 0.1384	
R indices (all data)	R_1 = 0.0844, wR_2 = 0.1481	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.695 and -1.918 $e.Å^{-3}$	

Table S3. Crystal data and structure refinement for **4-Sb.**

Identification code	4-Sb	
CCDC Number	2086627	
Empirical formula	$C_{29}H_{37}F_3O_4PSSb$	
Formula weight	691.36	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	*P* 21/*n*	
Unit cell dimensions	*a* = 10.277(4) Å	*α* = 90°
	b = 15.806(6) Å	*β* = 96.915(13)°
	c = 19.121(7) Å	*γ* = 90°
Volume	3083(2) $Å^3$	
Z	4	
Density (calculated)	1.489 mg/m^3	
Absorption coefficient	1.064 mm^{-1}	
F(000)	1408	
Crystal size	0.095 x 0.055 x 0.045 mm^3	
Theta range for data collection	2.376 to 24.999°	
Index ranges	-12<=h<=12, -18<=k<=18, -22<=l<=22	
Reflections collected	36134	
Independent reflections	5433 [R_{int} = 0.1417]	
Completeness to theta = 24.999°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.954 and 0.906	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5433 / 100 / 353	
Goodness-of-fit on F^2	1.015	
Final R indices [I>2sigma(I)]	R_1 = 0.0551, wR_2 = 0.1094	
R indices (all data)	R_1 = 0.1032, wR_2 = 0.1316	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.586 and -0.667 $e.Å^{-3}$	

Table S4. Crystal data and structure refinement for **4-Bi.**

Identification code	4-Bi	
CCDC Number	2086625	
Empirical formula	$C_{25}H_{37}BiF_3O_4PS$	
Formula weight	730.55	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	*P* -1	
Unit cell dimensions	*a* = 9.601(2) Å	α = 71.295(8)°
	b = 12.221(3) Å	β = 77.227(8)°
	c = 13.822(3) Å	γ = 82.243(8)°
Volume	1494.6(6) $Å^{-3}$	
Z	2	
Density (calculated)	1.623 mg/m^3	
Absorption coefficient	6.067 mm^{-1}	
F(000)	720	
Crystal size	0.055 x 0.045 x 0.035 mm^{-3}	
Theta range for data collection	2.440 to 24.998°	
Index ranges	-11<=h<=11, -14<=k<=14, -16<=l<=16	
Reflections collected	38738	
Independent reflections	5262 [R_{int} = 0.0714]	
Completeness to theta = 24.998°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.816 and 0.731	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5262 / 122 / 377	
Goodness-of-fit on F^2	1.029	
Final R indices [I>2sigma(I)]	R_1 = 0.0371, wR_2 = 0.0737	
R indices (all data)	R_1 = 0.0604, wR_2 = 0.0827	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.656 and -0.447 $e.Å^{-3}$	

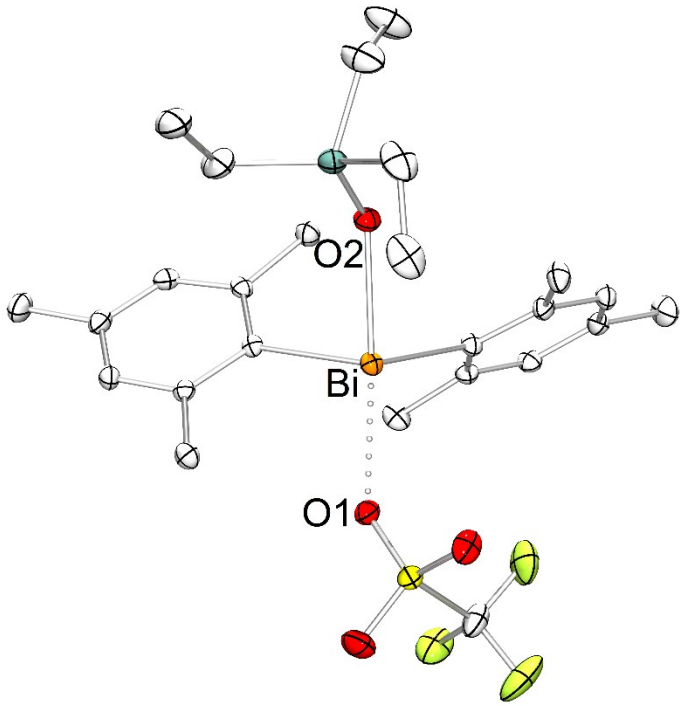


Figure S61: Solid-state structure of **4-Bi**. Thermal ellipsoids are drawn at 35% probability level and hydrogen atoms are omitted for clarity. Selected distances in **4-Bi**: Bi—O1 2.528(5), Bi—O2 2.349(4), P1—O2 1.491(5).

3. Computational Details

All the calculations are carried out using Gaussian 16 program package, Version-C.[11] Geometry optimization are carried out at B3LYP-D3 level of theory with Def2-TZVP basis set for Sb and Bi and 6-31G(d,p) basis set for all the other elements (C, H, O, P, F, S and Cl). The nature of stationary points is examined by vibrational frequency calculations at the same level of theory. Natural Bond Orbital (NBO) analysis is performed (using Gaussian 09, version-D program package[12]) to get the Natural Population Analysis (NPA) charges with the NBO6 method at the same level of theory.[13]

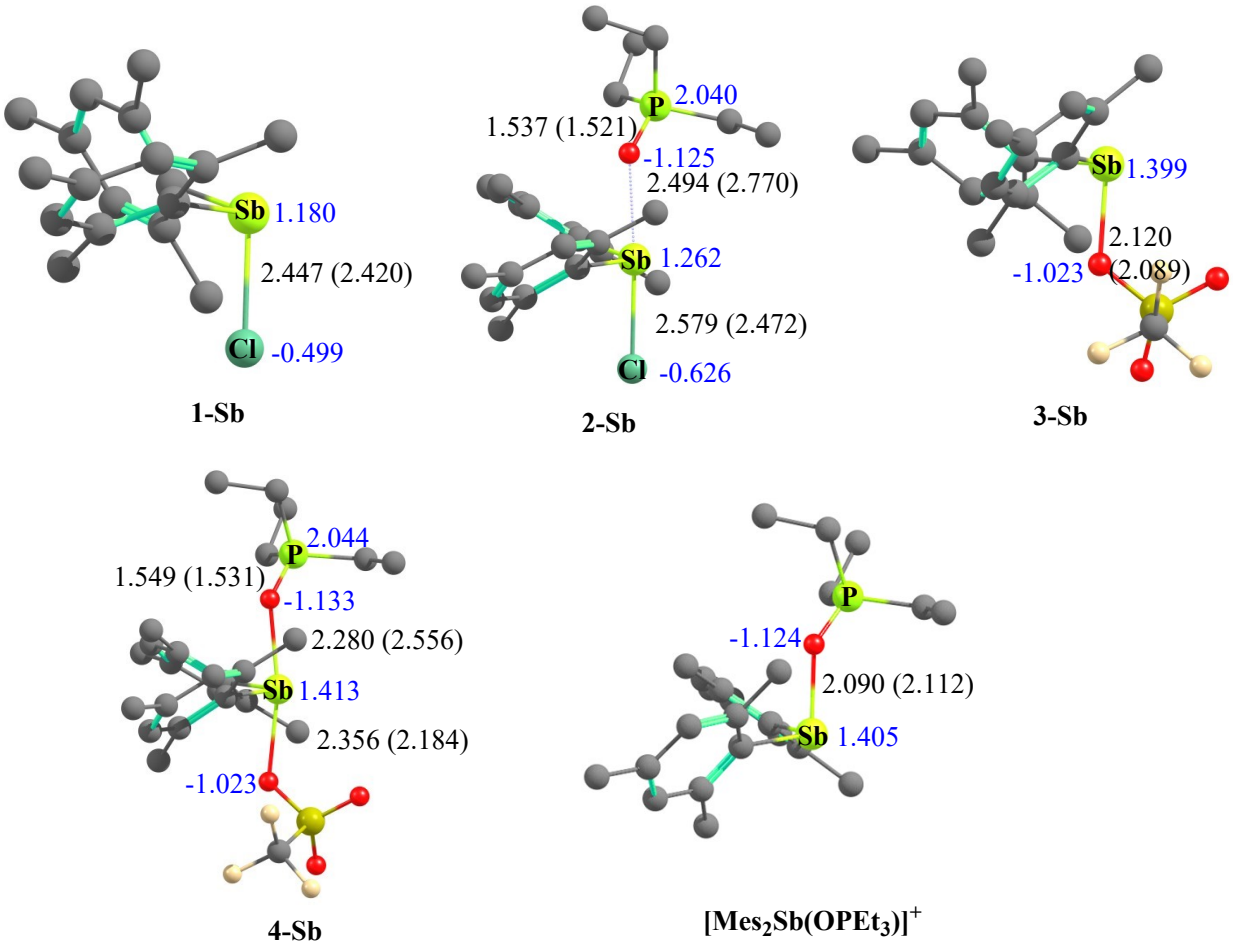


Figure S62: Important bond lengths (black) and NBO charges (blue) at B3LYP-D3 level of theory with the Def2-TZVP basis set for Sb and 6-31G(d, p) basis set for all other atoms with IEFPCM solvation model and dichloromethane solvent. Values in the parenthesis are bond lengths obtained from the gas phase calculation. H-atoms are not shown for simplicity.

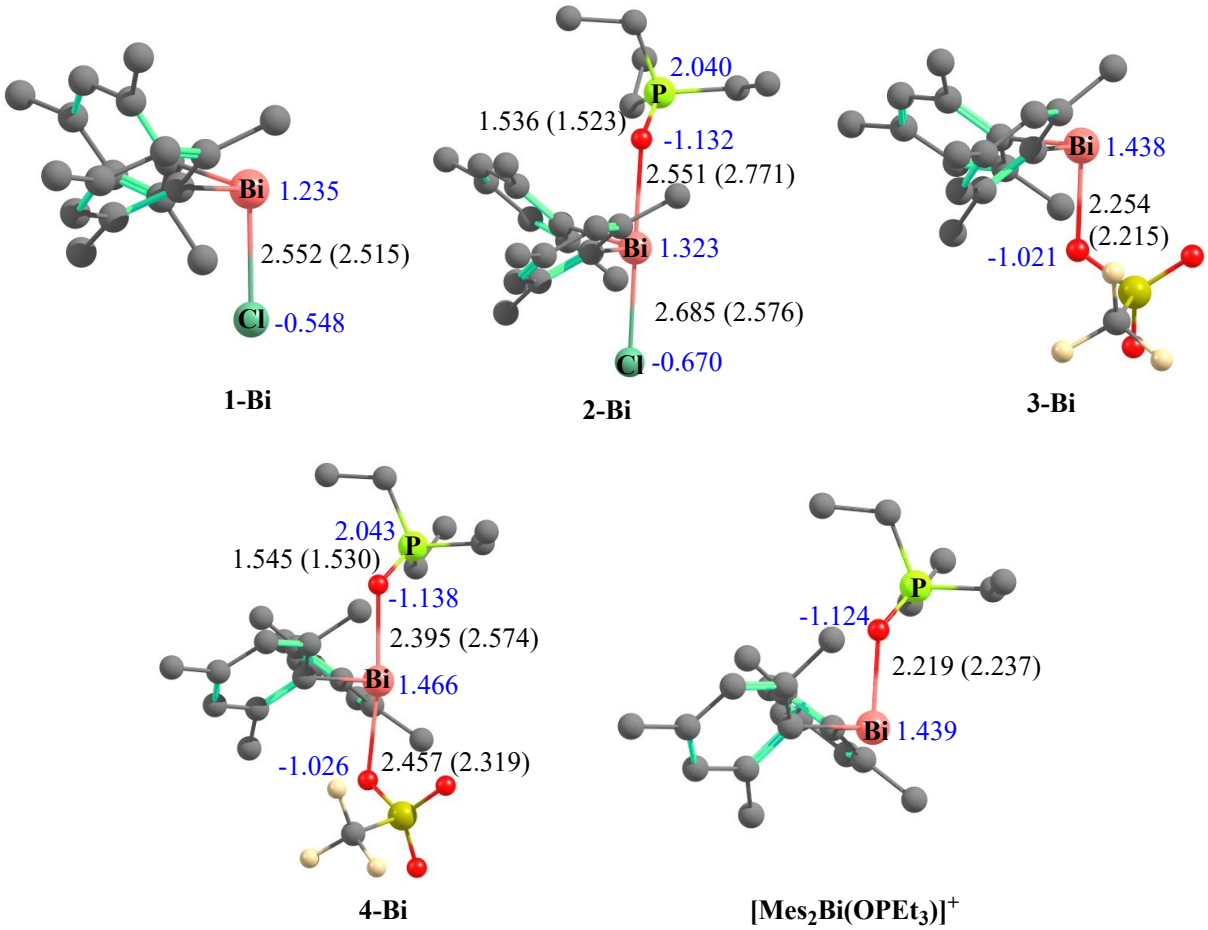


Figure S63: Important bond lengths (black) and NBO charges (blue) at B3LYP-D3 level of theory with the Def2-TZVP basis set for Bi and 6-31G(d, p) basis set for all other atoms with IEFPCM solvation model and dichloromethane solvent. Values in the parenthesis are bond lengths obtained from the gas phase calculation. H-atoms are not shown for simplicity.

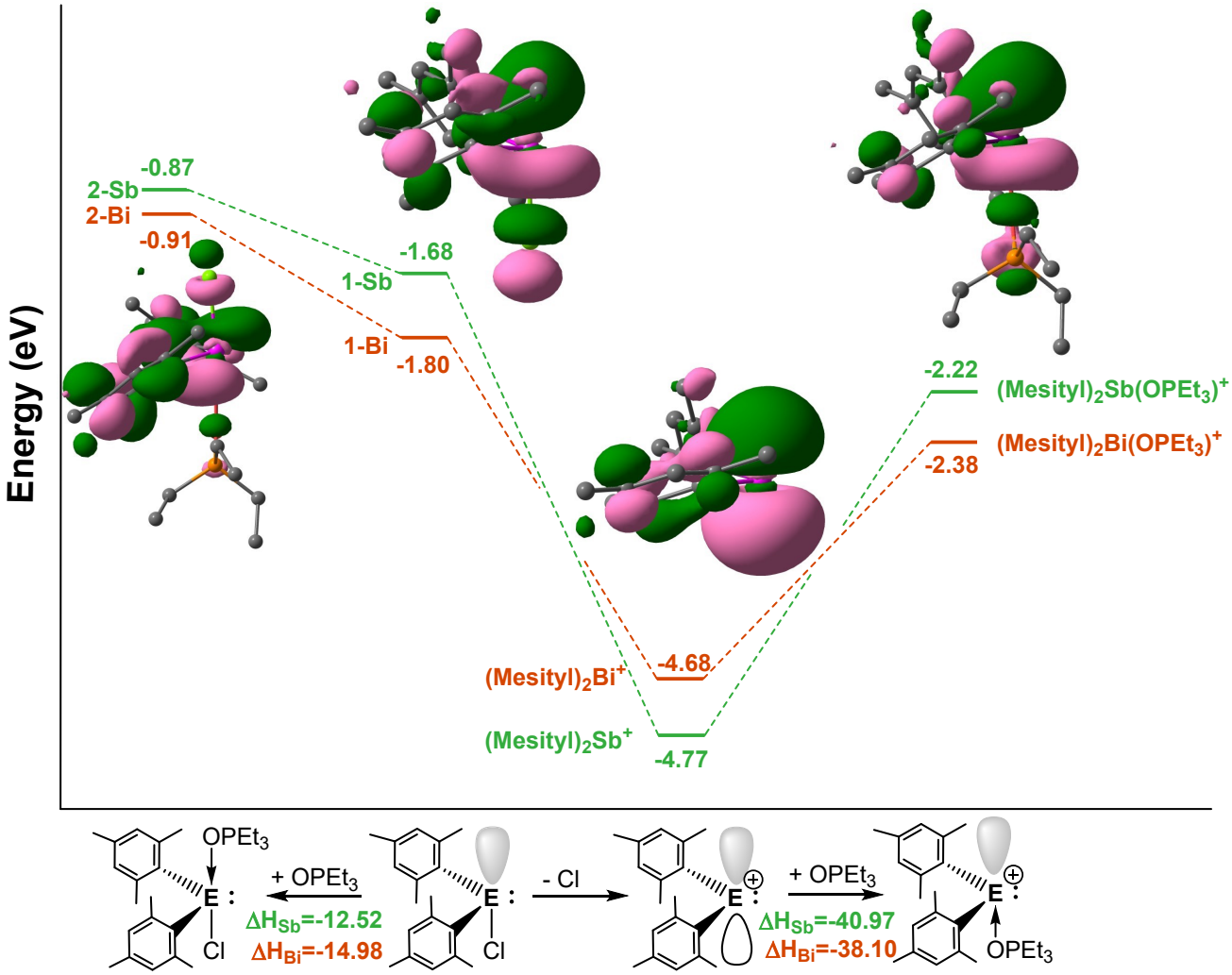


Figure S64: A schematic correlation diagram depicting the evolution of the acceptor orbitals (LUMO) of **1-Sb**, **1-Bi**, $[(Mesityl)_2Sb]^+$ and $[(Mesityl)_2Bi]^+$ and their interaction with $OPEt_3$ on either end. Energies of interaction, ΔH ($kcalmol^{-1}$), between the Lewis acids and $OPEt_3$, are provided below the arrows.

Cartesian coordinates of all the optimized geometries at B3LYP-D3 level of theory with the Def2-TZVP basis set for Bi and 6-31G (d, p) basis set for all other atoms with IEFPCM solvation model and dichloromethane solvent.

1-Sb

Total energy including ZPVE: -1399.472815 a. u.

Total electronic and thermal enthalpies: -1399.448372 a. u.

C	1.622630000	-0.026886000	-0.009837000
C	1.562282000	0.813520000	1.127441000
C	2.667560000	1.620925000	1.428463000
C	3.821909000	1.632515000	0.641901000
C	3.861639000	0.794941000	-0.475217000
C	2.785578000	-0.033255000	-0.815817000
C	0.354080000	0.918643000	2.033752000
C	4.980277000	2.541394000	0.975074000
C	2.921962000	-0.897129000	-2.056043000
C	-1.679394000	-0.027856000	-0.309558000
C	-1.619150000	1.230638000	-0.954618000
C	-2.690992000	2.121632000	-0.820801000
C	-3.829992000	1.802490000	-0.078078000
C	-3.896059000	0.532314000	0.498623000
C	-2.851813000	-0.395555000	0.387499000
C	-0.441387000	1.675478000	-1.800022000
C	-4.953391000	2.796346000	0.092404000
C	-3.050103000	-1.753731000	1.023847000
H	2.622382000	2.260752000	2.307206000
H	4.754119000	0.782177000	-1.096838000
H	-0.071728000	-0.057085000	2.274339000
H	0.623913000	1.409183000	2.972900000
H	-0.438222000	1.509615000	1.563904000
H	4.858347000	3.519796000	0.493793000
H	5.054566000	2.716480000	2.052501000
H	5.929958000	2.123937000	0.627582000
H	2.194324000	-0.623999000	-2.829777000
H	3.915583000	-0.783118000	-2.497000000
H	2.783389000	-1.961685000	-1.837755000
H	-2.636064000	3.086580000	-1.320465000

H	-4.793066000	0.245496000	1.043398000
H	0.382743000	2.047888000	-1.184507000
H	-0.037916000	0.868375000	-2.424090000
H	-0.741206000	2.476290000	-2.481199000
H	-4.791803000	3.417314000	0.982355000
H	-5.025357000	3.471229000	-0.765814000
H	-5.917455000	2.294279000	0.217328000
H	-4.110675000	-1.932043000	1.220695000
H	-2.690683000	-2.566500000	0.385021000
H	-2.513167000	-1.837313000	1.973017000
Sb	0.019166000	-1.363012000	-0.622780000
Cl	0.133927000	-2.648974000	1.455947000

2-Sb

Total energy including ZPVE: -2053.627354 a. u.

Total electronic and thermal enthalpies: -2053.589998 a. u.

C	2.346286000	0.000787000	-0.032096000
C	2.994235000	-1.001318000	0.726746000
C	4.162557000	-0.675641000	1.431256000
C	4.725258000	0.600487000	1.394957000
C	4.097827000	1.566256000	0.604403000
C	2.927763000	1.291639000	-0.114266000
C	2.533697000	-2.441227000	0.806423000
C	5.961213000	0.933236000	2.196179000
C	2.347954000	2.407785000	-0.962584000
C	-0.803319000	-1.481021000	0.058607000
C	-0.859708000	-1.395731000	1.472776000
C	-1.876011000	-2.077697000	2.157492000
C	-2.859510000	-2.818035000	1.500576000
C	-2.817936000	-2.855308000	0.105819000
C	-1.815268000	-2.202921000	-0.624710000
C	0.094873000	-0.581765000	2.322299000
C	-3.927945000	-3.555491000	2.270944000
C	-1.892428000	-2.290489000	-2.136239000
C	-2.028255000	3.743291000	0.778513000
C	-1.624171000	3.706792000	2.259691000

C	-3.152005000	1.012497000	0.838249000
C	-4.580803000	1.563551000	0.946965000
C	-2.527532000	2.288083000	-1.735664000
C	-1.578106000	3.126611000	-2.603905000
H	4.647627000	-1.450236000	2.022352000
H	4.532710000	2.561588000	0.539917000
H	3.018998000	-3.035935000	0.026443000
H	2.798949000	-2.875654000	1.775460000
H	1.460135000	-2.556195000	0.661080000
H	5.692676000	1.328735000	3.183919000
H	6.584355000	0.048618000	2.358478000
H	6.568982000	1.694401000	1.697155000
H	1.354547000	2.700972000	-0.613673000
H	2.996800000	3.287448000	-0.935310000
H	2.249978000	2.109662000	-2.013315000
H	-1.909637000	-2.005862000	3.242882000
H	-3.590865000	-3.399288000	-0.432994000
H	1.007939000	-1.138892000	2.550405000
H	0.385115000	0.347434000	1.835692000
H	-0.378139000	-0.331718000	3.276924000
H	-3.600161000	-4.573297000	2.516602000
H	-4.160386000	-3.052903000	3.214820000
H	-4.851825000	-3.643222000	1.691123000
H	-2.832699000	-2.752942000	-2.447728000
H	-1.843286000	-1.302415000	-2.609483000
H	-1.069081000	-2.879196000	-2.549875000
H	-3.040193000	4.142005000	0.647499000
H	-1.351027000	4.389447000	0.210036000
H	-0.626106000	3.276541000	2.380676000
H	-1.612335000	4.718779000	2.673531000
H	-2.325288000	3.111664000	2.853144000
H	-2.731927000	0.809474000	1.828001000
H	-3.135866000	0.056493000	0.305427000
H	-5.019838000	1.760504000	-0.035629000
H	-5.218383000	0.831793000	1.451211000
H	-4.618161000	2.490096000	1.527675000
H	-3.533072000	2.722051000	-1.714193000
H	-2.624203000	1.273254000	-2.139135000
H	-1.938276000	3.152918000	-3.636029000
H	-1.511794000	4.159093000	-2.247798000
H	-0.570582000	2.701831000	-2.605898000

O	-0.511539000	1.553235000	0.060299000
P	-1.947781000	2.096273000	-0.010656000
Sb	0.542578000	-0.310661000	-1.218600000
Cl	1.608229000	-2.346442000	-2.390466000

1-Bi

Total energy including ZPVE: -1373.848632 a. u.

Total electronic and thermal enthalpies: -1373.823830 a. u.

C	1.682409000	0.195729000	0.071905000
C	1.627601000	1.079072000	1.173246000
C	2.725935000	1.914712000	1.421222000
C	3.866023000	1.909529000	0.613442000
C	3.897939000	1.028435000	-0.470211000
C	2.826642000	0.172553000	-0.755709000
C	0.430556000	1.190909000	2.092614000
C	5.016873000	2.847924000	0.887310000
C	2.942544000	-0.737846000	-1.964046000
C	-1.741608000	0.192591000	-0.234200000
C	-1.672458000	1.413205000	-0.942707000
C	-2.744750000	2.311550000	-0.864253000
C	-3.887305000	2.034139000	-0.109681000
C	-3.953283000	0.803170000	0.547384000
C	-2.907407000	-0.128667000	0.492570000
C	-0.481153000	1.809483000	-1.792594000
C	-5.013028000	3.034943000	-0.004830000
C	-3.085648000	-1.440656000	1.223701000
H	2.686625000	2.590312000	2.273231000
H	4.778468000	1.003859000	-1.108735000
H	0.094202000	0.213468000	2.446354000
H	0.672087000	1.801702000	2.966689000
H	-0.416665000	1.657160000	1.580729000
H	4.875784000	3.801932000	0.363996000
H	5.104752000	3.072989000	1.954427000
H	5.967145000	2.427095000	0.545236000
H	2.199102000	-0.495584000	-2.733974000
H	3.925398000	-0.639533000	-2.432140000

H	2.815430000	-1.794505000	-1.701844000
H	-2.687252000	3.247998000	-1.415512000
H	-4.848614000	0.552764000	1.112761000
H	0.349310000	2.171650000	-1.179254000
H	-0.096216000	0.978010000	-2.396189000
H	-0.753570000	2.603069000	-2.493479000
H	-4.853612000	3.714025000	0.842056000
H	-5.086501000	3.651567000	-0.905785000
H	-5.976111000	2.540073000	0.152559000
H	-4.133952000	-1.594567000	1.493484000
H	-2.771555000	-2.296282000	0.616381000
H	-2.491955000	-1.472625000	2.141699000
Bi	0.014586000	-1.254040000	-0.488255000
Cl	0.132812000	-2.437287000	1.770088000

2-Bi

Total energy including ZPVE: -2028.007129 a. u.

Total electronic and thermal enthalpies: -2027.969382 a. u.

C	2.386693000	0.121848000	0.177370000
C	3.050441000	-0.909903000	0.877911000
C	4.189204000	-0.594308000	1.634015000
C	4.699682000	0.703272000	1.707434000
C	4.047330000	1.703735000	0.983008000
C	2.905172000	1.436683000	0.216246000
C	2.621263000	-2.360619000	0.839567000
C	5.904948000	1.019527000	2.560979000
C	2.273563000	2.587796000	-0.543172000
C	-0.792152000	-1.525096000	0.182192000
C	-0.900946000	-1.365630000	1.584862000
C	-1.932232000	-2.028554000	2.268148000
C	-2.862141000	-2.840864000	1.614938000
C	-2.744585000	-2.979804000	0.230862000
C	-1.733810000	-2.334627000	-0.494785000
C	0.030074000	-0.506601000	2.413784000
C	-3.946829000	-3.557484000	2.382802000
C	-1.727806000	-2.509765000	-1.999814000
C	-2.609253000	3.085770000	1.534474000

C	-2.477207000	2.297580000	2.845666000
C	-3.397485000	0.707679000	-0.021739000
C	-4.879427000	1.103524000	0.046493000
C	-2.527038000	3.147049000	-1.407072000
C	-1.497519000	4.273958000	-1.574860000
H	4.692451000	-1.391145000	2.178563000
H	4.436950000	2.719469000	1.012230000
H	3.003964000	-2.850137000	-0.060890000
H	3.003842000	-2.900407000	1.710948000
H	1.535931000	-2.475912000	0.816440000
H	5.603121000	1.296796000	3.578940000
H	6.574198000	0.157790000	2.644459000
H	6.476181000	1.858849000	2.152420000
H	1.250295000	2.776415000	-0.206033000
H	2.851603000	3.506116000	-0.408709000
H	2.232766000	2.389235000	-1.621657000
H	-2.014093000	-1.895566000	3.345175000
H	-3.467225000	-3.593270000	-0.303415000
H	0.998106000	-0.992170000	2.563838000
H	0.219662000	0.457675000	1.941815000
H	-0.401905000	-0.324789000	3.402040000
H	-3.606278000	-4.547942000	2.709562000
H	-4.236308000	-3.001782000	3.279997000
H	-4.839882000	-3.707971000	1.768516000
H	-2.557441000	-3.144673000	-2.321759000
H	-1.837500000	-1.549907000	-2.521824000
H	-0.796156000	-2.959408000	-2.353335000
H	-3.623613000	3.479534000	1.406186000
H	-1.929354000	3.944407000	1.529354000
H	-1.459977000	1.921427000	2.975296000
H	-2.714255000	2.941738000	3.696885000
H	-3.159004000	1.441853000	2.873670000
H	-3.134476000	0.024155000	0.790787000
H	-3.179891000	0.169391000	-0.949922000
H	-5.165664000	1.773879000	-0.769354000
H	-5.500937000	0.206748000	-0.028899000
H	-5.124497000	1.595020000	0.992789000
H	-3.543933000	3.546571000	-1.327397000
H	-2.510681000	2.478151000	-2.275720000
H	-1.704955000	4.840614000	-2.486812000
H	-1.524254000	4.974167000	-0.734265000

H	-0.484349000	3.869489000	-1.646772000
O	-0.743998000	1.617321000	0.093098000
P	-2.204380000	2.092317000	0.053859000
Bi	0.547457000	-0.203042000	-1.142819000
Cl	1.808037000	-2.150369000	-2.494571000

$[(Mesityl)_2Sb]^+$

Total energy including ZPVE: -939.035342 a. u.

Total electronic and thermal enthalpies: -939.012966 a. u.

C	1.644268000	-0.233894000	0.126115000
C	1.675668000	0.886995000	1.009571000
C	2.845398000	1.635311000	1.081880000
C	3.983222000	1.331265000	0.311974000
C	3.939129000	0.221164000	-0.533842000
C	2.795375000	-0.574440000	-0.637245000
C	0.512541000	1.289447000	1.892838000
C	5.215792000	2.187359000	0.421474000
C	2.805976000	-1.720418000	-1.622482000
C	-1.634913000	-0.199933000	-0.120437000
C	-1.633016000	0.974294000	-0.936476000
C	-2.804260000	1.719926000	-1.018434000
C	-3.974340000	1.368541000	-0.321983000
C	-3.961529000	0.212997000	0.463164000
C	-2.820481000	-0.583184000	0.572196000
C	-0.439987000	1.443714000	-1.743308000
C	-5.204706000	2.226252000	-0.436850000
C	-2.870895000	-1.784808000	1.488001000
H	2.888448000	2.479056000	1.765897000
H	4.811938000	-0.028937000	-1.130713000
H	0.059140000	0.436444000	2.407744000
H	0.846769000	1.990039000	2.661183000
H	-0.278774000	1.780153000	1.319250000
H	4.989879000	3.224854000	0.150350000
H	5.585029000	2.202073000	1.453106000
H	6.018721000	1.829209000	-0.226509000
H	2.389588000	-1.411309000	-2.588072000

H	3.823710000	-2.075399000	-1.800801000
H	2.219627000	-2.582695000	-1.278132000
H	-2.821341000	2.602008000	-1.653250000
H	-4.858807000	-0.072125000	1.005289000
H	0.326275000	1.893949000	-1.106575000
H	0.037872000	0.634883000	-2.303202000
H	-0.752110000	2.198700000	-2.468055000
H	-5.015145000	3.225181000	-0.027076000
H	-5.485174000	2.362169000	-1.487078000
H	-6.054072000	1.793141000	0.095871000
H	-3.901945000	-2.101082000	1.661712000
H	-2.334442000	-2.650854000	1.079363000
H	-2.427842000	-1.555640000	2.463661000
Sb	-0.009937000	-1.540732000	0.000570000

$[(Mesityl)_2Sb(OPEt_3)]^+$

Total energy including ZPVE: -1593.234942 a. u.

Total electronic and thermal enthalpies: -1593.199933 a. u.

C	2.322716000	0.101790000	-0.360726000
C	3.060871000	-1.103327000	-0.392580000
C	4.328514000	-1.140737000	0.197346000
C	4.890682000	-0.015773000	0.808415000
C	4.163928000	1.176956000	0.782155000
C	2.893076000	1.265616000	0.198512000
C	2.529860000	-2.367970000	-1.036795000
C	6.242073000	-0.090697000	1.476312000
C	2.200403000	2.611970000	0.207690000
C	-0.589654000	-1.549299000	-0.322138000
C	-0.513966000	-1.760770000	1.076691000
C	-1.355490000	-2.718029000	1.657474000
C	-2.255376000	-3.478303000	0.904418000
C	-2.296636000	-3.270650000	-0.476581000
C	-1.479283000	-2.323423000	-1.104285000
C	0.442283000	-1.023169000	1.990088000
C	-3.130946000	-4.515972000	1.562330000
C	-1.592471000	-2.167948000	-2.609567000

C	-1.925601000	3.043257000	1.672765000
C	-1.493955000	2.340019000	2.968306000
C	-3.125088000	0.560084000	0.552702000
C	-4.539885000	1.000210000	0.960985000
C	-2.554061000	2.866353000	-1.223636000
C	-1.622192000	4.018114000	-1.630863000
H	4.893951000	-2.069556000	0.170442000
H	4.601810000	2.071969000	1.218445000
H	2.050774000	-2.179217000	-2.006757000
H	3.340420000	-3.076593000	-1.224241000
H	1.789822000	-2.865091000	-0.401617000
H	6.142963000	-0.430946000	2.514497000
H	6.902168000	-0.797928000	0.965249000
H	6.733794000	0.886069000	1.497980000
H	1.438649000	2.665109000	0.990778000
H	2.923093000	3.412845000	0.383107000
H	1.694967000	2.825285000	-0.740112000
H	-1.305888000	-2.873763000	2.732777000
H	-2.984974000	-3.857042000	-1.080485000
H	1.461779000	-1.406096000	1.879705000
H	0.480720000	0.045907000	1.779300000
H	0.148457000	-1.152667000	3.034813000
H	-2.601541000	-5.473237000	1.643043000
H	-3.414010000	-4.215423000	2.575462000
H	-4.043228000	-4.694588000	0.986194000
H	-2.291499000	-2.899913000	-3.021201000
H	-1.958173000	-1.175090000	-2.897439000
H	-0.630889000	-2.321905000	-3.112264000
H	-2.920517000	3.491760000	1.769405000
H	-1.231298000	3.849934000	1.416555000
H	-0.494361000	1.909749000	2.870672000
H	-1.472728000	3.064615000	3.785786000
H	-2.186428000	1.540801000	3.247386000
H	-2.661112000	-0.058738000	1.326600000
H	-3.146244000	-0.053689000	-0.353469000
H	-5.020365000	1.608429000	0.189753000
H	-5.158030000	0.112631000	1.116319000
H	-4.534507000	1.568436000	1.895268000
H	-3.560922000	3.231951000	-0.995091000
H	-2.657018000	2.136968000	-2.034893000
H	-1.999144000	4.484964000	-2.543994000

H	-1.571641000	4.789455000	-0.857644000
H	-0.607559000	3.661522000	-1.827704000
O	-0.504051000	1.425541000	0.017833000
P	-1.976073000	1.936944000	0.231435000
Sb	0.390655000	0.098721000	-1.326685000

[(Mesityl)$_2$Bi]$^+$

Total energy including ZPVE: -913.413829 a. u.

Total electronic and thermal enthalpies: -913.391071 a. u.

C	1.709473000	0.003247000	0.150285000
C	1.741901000	1.102338000	1.049310000
C	2.899536000	1.875377000	1.104521000
C	4.020179000	1.606400000	0.299618000
C	3.970748000	0.511100000	-0.564177000
C	2.835556000	-0.302725000	-0.650990000
C	0.585811000	1.459498000	1.959781000
C	5.238157000	2.489164000	0.379398000
C	2.835183000	-1.436575000	-1.651364000
C	-1.697180000	0.053680000	-0.175652000
C	-1.630229000	1.264634000	-0.923654000
C	-2.764096000	2.073619000	-0.976205000
C	-3.957499000	1.738858000	-0.317202000
C	-4.013062000	0.531388000	0.385709000
C	-2.912138000	-0.323458000	0.462708000
C	-0.404527000	1.718983000	-1.687884000
C	-5.141518000	2.666859000	-0.363416000
C	-3.053514000	-1.596683000	1.270465000
H	2.943092000	2.708306000	1.802041000
H	4.831598000	0.284360000	-1.187884000
H	0.220257000	0.595084000	2.524990000
H	0.890571000	2.212858000	2.689665000
H	-0.260999000	1.864607000	1.398436000
H	5.015527000	3.488149000	-0.013763000
H	5.560424000	2.619788000	1.417821000
H	6.073529000	2.079315000	-0.193207000
H	2.370896000	-1.131953000	-2.596175000

H	3.852463000	-1.765059000	-1.877756000
H	2.291722000	-2.320340000	-1.288105000
H	-2.727051000	2.991582000	-1.557236000
H	-4.936278000	0.250386000	0.885301000
H	0.351273000	2.143961000	-1.021672000
H	0.071259000	0.905333000	-2.241566000
H	-0.676920000	2.490109000	-2.412098000
H	-5.012138000	3.480861000	0.360807000
H	-5.247327000	3.128160000	-1.349797000
H	-6.071121000	2.148120000	-0.116147000
H	-4.106276000	-1.824235000	1.452699000
H	-2.626176000	-2.468850000	0.760682000
H	-2.569312000	-1.508075000	2.248982000
Bi	-0.021876000	-1.385382000	0.021765000

$[(Mesityl)_2Bi(OPEt_3)]^+$

Total energy including ZPVE: -1567.608799 a. u.

Total electronic and thermal enthalpies: -1567.573458 a. u.

C	2.370971000	0.005525000	-0.196603000
C	3.051331000	-1.228886000	-0.107003000
C	4.292120000	-1.272499000	0.538706000
C	4.879177000	-0.128553000	1.089690000
C	4.206837000	1.087487000	0.949421000
C	2.964592000	1.181704000	0.306137000
C	2.491163000	-2.515438000	-0.678525000
C	6.199265000	-0.210939000	1.817153000
C	2.320854000	2.547434000	0.191382000
C	-0.722098000	-1.593705000	-0.205686000
C	-0.674699000	-1.788598000	1.193892000
C	-1.569549000	-2.698242000	1.774439000
C	-2.495006000	-3.422584000	1.017224000
C	-2.508051000	-3.229190000	-0.366948000
C	-1.636287000	-2.329710000	-0.992253000
C	0.306046000	-1.083694000	2.106542000
C	-3.429209000	-4.410072000	1.672654000
C	-1.716136000	-2.179685000	-2.500018000

C	-1.936106000	2.996444000	1.976018000
C	-1.425057000	2.212972000	3.194234000
C	-3.177131000	0.645285000	0.639679000
C	-4.612328000	1.084725000	0.968611000
C	-2.543971000	3.072763000	-0.923846000
C	-1.546349000	4.184561000	-1.282990000
H	4.817458000	-2.222748000	0.605678000
H	4.663913000	1.993440000	1.341532000
H	2.134992000	-2.396243000	-1.709461000
H	3.255767000	-3.295976000	-0.700164000
H	1.649532000	-2.888560000	-0.086586000
H	6.048187000	-0.501666000	2.864097000
H	6.858406000	-0.958854000	1.365975000
H	6.718965000	0.751444000	1.816480000
H	1.502495000	2.667209000	0.906502000
H	3.053842000	3.336790000	0.376257000
H	1.899572000	2.721940000	-0.805641000
H	-1.541704000	-2.843388000	2.852193000
H	-3.216418000	-3.788038000	-0.974235000
H	1.304890000	-1.523928000	2.023032000
H	0.405414000	-0.024270000	1.869144000
H	-0.009867000	-1.170107000	3.149411000
H	-2.963009000	-5.400944000	1.736492000
H	-3.683497000	-4.104421000	2.691808000
H	-4.356694000	-4.522481000	1.103687000
H	-2.442935000	-2.877583000	-2.922745000
H	-2.029041000	-1.171850000	-2.800651000
H	-0.754583000	-2.386479000	-2.984456000
H	-2.947218000	3.384298000	2.141838000
H	-1.291625000	3.857095000	1.769367000
H	-0.402027000	1.864321000	3.036457000
H	-1.431765000	2.861185000	4.073998000
H	-2.052715000	1.344436000	3.414017000
H	-2.775645000	-0.016781000	1.412613000
H	-3.145185000	0.072086000	-0.292404000
H	-5.039166000	1.714149000	0.183007000
H	-5.244595000	0.198202000	1.062588000
H	-4.665772000	1.630347000	1.914861000
H	-3.517585000	3.488032000	-0.641849000
H	-2.716071000	2.408201000	-1.778704000
H	-1.917133000	4.745459000	-2.144400000

H	-1.413004000	4.890020000	-0.458136000
H	-0.567457000	3.772129000	-1.541857000
O	-0.533404000	1.486284000	0.189128000
P	-1.984357000	2.010615000	0.447011000
Bi	0.377128000	0.081704000	-1.267222000

3-Sb

Total energy including ZPVE: -1900.655515 a. u.

Total electronic and thermal enthalpies: -1900.624148 a. u.

C	-0.818710000	1.440245000	0.275431000
C	-0.894412000	1.647716000	-1.122256000
C	-1.723886000	2.668144000	-1.605862000
C	-2.473798000	3.487289000	-0.758662000
C	-2.381261000	3.268060000	0.618524000
C	-1.568661000	2.262074000	1.150965000
C	-0.141989000	0.818539000	-2.140224000
C	-3.331418000	4.599579000	-1.310964000
C	-1.509209000	2.118141000	2.660330000
C	2.273271000	0.088251000	0.310386000
C	2.850153000	1.359987000	0.076329000
C	4.135267000	1.428802000	-0.472854000
C	4.872081000	0.283452000	-0.789448000
C	4.305221000	-0.959767000	-0.503476000
C	3.025407000	-1.082775000	0.052790000
C	2.152321000	2.667024000	0.394250000
C	6.238561000	0.391240000	-1.421009000
C	2.518788000	-2.479398000	0.349269000
C	-2.811010000	-1.942774000	-0.738383000
H	-1.782987000	2.826240000	-2.680506000
H	-2.954303000	3.897328000	1.295629000
H	-0.676474000	-0.111075000	-2.351527000
H	-0.039277000	1.369474000	-3.078874000
H	0.856839000	0.543487000	-1.796923000
H	-2.764449000	5.537376000	-1.362963000
H	-3.679572000	4.372404000	-2.322714000
H	-4.204867000	4.782767000	-0.678097000

H	-0.512557000	2.350700000	3.055830000
H	-2.208984000	2.805810000	3.141609000
H	-1.767930000	1.106736000	2.993206000
H	4.577455000	2.406916000	-0.649184000
H	4.877131000	-1.862636000	-0.705780000
H	1.416950000	2.928018000	-0.372294000
H	1.619200000	2.641950000	1.350087000
H	2.879376000	3.481191000	0.452262000
H	6.155939000	0.465069000	-2.512452000
H	6.770224000	1.282902000	-1.075199000
H	6.853769000	-0.485430000	-1.198668000
H	3.354716000	-3.177693000	0.439867000
H	1.955005000	-2.528751000	1.288252000
H	1.857983000	-2.845855000	-0.441359000
O	-0.267408000	-1.512904000	-0.289945000
O	-1.490131000	-2.980445000	1.340494000
O	-0.892765000	-3.799421000	-0.982889000
S	-1.243914000	-2.707446000	-0.078395000
F	-3.105168000	-0.851839000	-0.023540000
F	-3.808540000	-2.822000000	-0.639810000
F	-2.645934000	-1.599339000	-2.019018000
Sb	0.318791000	-0.138235000	1.213987000

3-Bi

Total energy including ZPVE: -1875.030903 a. u.

Total electronic and thermal enthalpies: -1874.999161 a. u.

C	0.915150000	1.481388000	-0.175011000
C	0.999852000	1.683038000	1.220435000
C	1.879933000	2.660890000	1.704410000
C	2.672701000	3.437835000	0.856037000
C	2.574361000	3.217929000	-0.520880000
C	1.710911000	2.253018000	-1.051446000
C	0.206803000	0.883340000	2.230413000
C	3.585214000	4.506504000	1.407430000
C	1.661245000	2.084169000	-2.558630000
C	-2.345240000	0.143954000	-0.137673000

C	-2.889658000	1.419079000	0.143380000
C	-4.151506000	1.497792000	0.744264000
C	-4.893898000	0.357434000	1.067290000
C	-4.356840000	-0.888875000	0.740488000
C	-3.099801000	-1.020177000	0.133994000
C	-2.177704000	2.715882000	-0.182597000
C	-6.233243000	0.474338000	1.753556000
C	-2.616880000	-2.417728000	-0.196753000
C	2.820147000	-1.939449000	1.019912000
H	1.946712000	2.817132000	2.779024000
H	3.183849000	3.811824000	-1.198472000
H	0.671052000	-0.091162000	2.401979000
H	0.162531000	1.409330000	3.187808000
H	-0.816546000	0.696494000	1.898262000
H	3.066852000	5.472069000	1.459472000
H	3.921998000	4.262645000	2.419250000
H	4.466986000	4.645069000	0.774653000
H	0.668634000	2.307238000	-2.968940000
H	2.363508000	2.762548000	-3.049501000
H	1.929727000	1.067203000	-2.869183000
H	-4.570384000	2.478760000	0.958115000
H	-4.932925000	-1.786826000	0.953163000
H	-1.313384000	2.878459000	0.466752000
H	-1.813852000	2.743004000	-1.215905000
H	-2.853600000	3.566058000	-0.059692000
H	-6.107583000	0.534264000	2.841770000
H	-6.766908000	1.376470000	1.439161000
H	-6.867944000	-0.391924000	1.545479000
H	-3.451118000	-3.123833000	-0.195164000
H	-2.152947000	-2.472546000	-1.189211000
H	-1.873840000	-2.769946000	0.523995000
O	0.293206000	-1.598152000	0.421486000
O	1.714623000	-2.803119000	-1.247757000
O	1.021826000	-3.914265000	0.919530000
S	1.346913000	-2.700075000	0.171260000
F	3.119260000	-0.773310000	0.438301000
F	3.865799000	-2.763634000	0.923413000
F	2.543982000	-1.726633000	2.311619000
Bi	-0.337100000	-0.125263000	-1.164346000

4-Sb

Total energy including ZPVE: -2554.819832 a. u.

Total electronic and thermal enthalpies: -2554.775615 a. u.

C	1.149056000	1.337967000	0.613809000
C	1.819320000	1.005597000	1.814229000
C	2.540216000	2.001345000	2.489168000
C	2.644441000	3.306505000	2.008168000
C	2.014862000	3.605775000	0.797829000
C	1.277624000	2.649303000	0.089879000
C	1.865684000	-0.382057000	2.417759000
C	3.399797000	4.364714000	2.775820000
C	0.655091000	3.081625000	-1.223525000
C	-1.063768000	-1.332848000	0.778430000
C	-1.681100000	-0.861066000	1.963560000
C	-2.539451000	-1.714783000	2.670562000
C	-2.818191000	-3.015709000	2.246815000
C	-2.209773000	-3.461842000	1.072295000
C	-1.340082000	-2.649735000	0.331912000
C	-1.469622000	0.523437000	2.541579000
C	-3.732298000	-3.915953000	3.042324000
C	-0.740813000	-3.239349000	-0.930000000
C	4.363944000	-0.930349000	-0.574842000
C	-4.106244000	2.702584000	-0.762973000
C	-4.220618000	3.011329000	0.737586000
C	-4.132369000	-0.229128000	-0.346025000
C	-5.591835000	-0.358810000	-0.806172000
C	-3.157193000	0.877827000	-2.896994000
C	-2.321237000	1.919166000	-3.655652000
H	3.044513000	1.739073000	3.417287000
H	2.104616000	4.609621000	0.387906000
H	2.756049000	-0.910751000	2.067271000
H	1.918574000	-0.322034000	3.509317000
H	1.010227000	-0.998348000	2.147850000
H	2.730600000	4.907344000	3.455385000
H	4.196249000	3.926572000	3.384771000
H	3.847713000	5.103409000	2.104010000
H	-0.432633000	3.156929000	-1.145793000
H	1.045151000	4.054864000	-1.532574000

H	0.872999000	2.373673000	-2.031808000
H	-3.013070000	-1.343678000	3.577331000
H	-2.421546000	-4.467384000	0.715192000
H	-0.567431000	0.556340000	3.160475000
H	-1.365295000	1.285688000	1.771970000
H	-2.313310000	0.798192000	3.181676000
H	-3.164800000	-4.487576000	3.787154000
H	-4.490127000	-3.340742000	3.582858000
H	-4.242484000	-4.638741000	2.398436000
H	-1.233632000	-4.180189000	-1.188141000
H	-0.844164000	-2.569557000	-1.791408000
H	0.327890000	-3.436036000	-0.808833000
H	-5.091448000	2.631545000	-1.236148000
H	-3.555633000	3.495135000	-1.280376000
H	-3.232969000	3.054368000	1.204273000
H	-4.710620000	3.977527000	0.883316000
H	-4.812421000	2.254140000	1.260946000
H	-4.067875000	-0.093245000	0.737541000
H	-3.564609000	-1.139482000	-0.563684000
H	-5.668541000	-0.529890000	-1.883841000
H	-6.056235000	-1.211298000	-0.303145000
H	-6.179050000	0.530528000	-0.559125000
H	-4.190313000	0.856248000	-3.260205000
H	-2.744359000	-0.127478000	-3.041102000
H	-2.299173000	1.671782000	-4.720185000
H	-2.739053000	2.925242000	-3.555586000
H	-1.291257000	1.939322000	-3.290978000
O	1.837834000	-1.565380000	-0.283466000
O	2.670215000	-1.122314000	-2.602983000
O	3.311184000	-3.232389000	-1.384078000
O	-1.777596000	1.291007000	-0.499190000
P	-3.201829000	1.153655000	-1.091869000
S	2.912472000	-1.819121000	-1.327355000
F	4.086715000	0.371079000	-0.426054000
F	5.436012000	-1.056878000	-1.367617000
F	4.656142000	-1.447997000	0.628767000
Sb	0.044898000	-0.074245000	-0.616817000

4-Bi

Total energy including ZPVE: -2529.198951 a. u.

Total electronic and thermal enthalpies: -2529.154373 a. u.

C	1.254243000	1.371003000	0.701514000
C	1.920721000	1.021743000	1.896044000
C	2.666414000	2.002181000	2.567648000
C	2.789190000	3.306364000	2.086271000
C	2.150773000	3.622294000	0.883919000
C	1.391918000	2.678889000	0.180521000
C	1.925194000	-0.371279000	2.487558000
C	3.571120000	4.349624000	2.848372000
C	0.748511000	3.112789000	-1.122143000
C	-1.144225000	-1.275088000	0.950483000
C	-1.758644000	-0.683828000	2.079110000
C	-2.693877000	-1.429855000	2.812000000
C	-3.041541000	-2.738191000	2.466200000
C	-2.423829000	-3.304628000	1.349013000
C	-1.485353000	-2.598039000	0.585059000
C	-1.462323000	0.721466000	2.557837000
C	-4.036229000	-3.522468000	3.287869000
C	-0.892909000	-3.288177000	-0.628170000
C	4.402804000	-0.979062000	-0.555228000
C	-4.314540000	2.531194000	-0.593152000
C	-4.469505000	2.572213000	0.934473000
C	-4.043736000	-0.412695000	-0.643603000
C	-5.513591000	-0.578069000	-1.056902000
C	-3.243396000	1.172778000	-2.991420000
C	-2.472659000	2.366258000	-3.574791000
H	3.172662000	1.730449000	3.492053000
H	2.249359000	4.627636000	0.479285000
H	2.754647000	-0.952563000	2.076140000
H	2.049325000	-0.327875000	3.573898000
H	1.013274000	-0.927646000	2.269039000
H	2.917008000	4.911385000	3.527090000
H	4.358466000	3.895196000	3.457231000
H	4.035268000	5.074612000	2.172538000
H	-0.342591000	3.117080000	-1.048996000
H	1.076006000	4.117317000	-1.402519000

H	1.016397000	2.445209000	-1.950970000
H	-3.169129000	-0.968995000	3.675754000
H	-2.686518000	-4.318910000	1.055661000
H	-0.513231000	0.762600000	3.100745000
H	-1.392815000	1.429355000	1.732030000
H	-2.246233000	1.065987000	3.238396000
H	-3.529913000	-4.083296000	4.083323000
H	-4.766158000	-2.864227000	3.768791000
H	-4.578801000	-4.248196000	2.674386000
H	-1.313461000	-4.289498000	-0.750964000
H	-1.102283000	-2.737041000	-1.554332000
H	0.193428000	-3.382344000	-0.548260000
H	-5.285726000	2.441693000	-1.092145000
H	-3.846867000	3.450535000	-0.961067000
H	-3.496891000	2.652957000	1.425892000
H	-5.072119000	3.436661000	1.225486000
H	-4.967531000	1.674628000	1.313891000
H	-3.927628000	-0.473530000	0.442642000
H	-3.427094000	-1.218023000	-1.055763000
H	-5.644594000	-0.533570000	-2.142069000
H	-5.878527000	-1.551961000	-0.719379000
H	-6.150616000	0.187709000	-0.604589000
H	-4.279829000	1.155957000	-3.345052000
H	-2.782167000	0.227227000	-3.300060000
H	-2.451879000	2.299618000	-4.665784000
H	-2.939553000	3.319066000	-3.307526000
H	-1.440888000	2.380042000	-3.214082000
O	1.906130000	-1.711940000	-0.226573000
O	2.675687000	-1.217890000	-2.549378000
O	3.430071000	-3.312533000	-1.367752000
O	-1.837287000	1.327408000	-0.591601000
P	-3.261663000	1.154568000	-1.164242000
S	2.972660000	-1.918628000	-1.284911000
F	4.091429000	0.317558000	-0.428774000
F	5.476339000	-1.090310000	-1.348260000
F	4.711013000	-1.466585000	0.656871000
Bi	0.083211000	-0.103091000	-0.580548000

$OPEt_3$

Total energy including ZPVE: -654.134097 a. u.

Total electronic and thermal enthalpies: -654.121674 a. u.

C	0.483605000	-1.200410000	-0.846977000
C	1.774730000	-1.912798000	-0.421679000
C	1.132918000	1.232241000	0.667230000
C	1.667924000	1.913843000	-0.600224000
C	-1.565753000	0.820047000	-0.371927000
C	-2.772904000	-0.091638000	-0.632168000
H	0.628146000	-0.643606000	-1.779796000
H	-0.311727000	-1.930567000	-1.032620000
H	1.635749000	-2.442977000	0.524948000
H	2.077394000	-2.643203000	-1.177618000
H	2.600732000	-1.205771000	-0.293899000
H	1.945879000	0.741219000	1.213667000
H	0.701088000	1.970097000	1.353235000
H	0.875186000	2.425350000	-1.154142000
H	2.420473000	2.662906000	-0.336643000
H	2.141737000	1.195487000	-1.275968000
H	-1.211259000	1.275124000	-1.303533000
H	-1.843111000	1.640603000	0.300233000
H	-3.610112000	0.486914000	-1.033504000
H	-2.535392000	-0.876990000	-1.356525000
H	-3.103937000	-0.573885000	0.291838000
O	-0.538224000	-0.737380000	1.727796000
P	-0.161879000	-0.049958000	0.431495000

Cartesian coordinates of all the optimized geometries at B3LYP-D3 level of theory with the Def2-TZVP basis set for Bi and 6-31G(d,p) basis set for all other atoms. (Gas phase calculation)

1-Sb (g)

Total energy including ZPVE: -1399.466885 a. u.

Total electronic and thermal enthalpies: -1399.442470 a. u.

C	1.610631000	-0.030268000	0.008737000
C	1.540243000	0.766301000	1.176059000
C	2.620244000	1.602935000	1.486623000
C	3.760112000	1.682795000	0.684554000
C	3.812760000	0.884196000	-0.459182000
C	2.761440000	0.030124000	-0.810858000
C	0.350744000	0.779155000	2.111598000
C	4.889900000	2.622099000	1.031537000
C	2.911636000	-0.793233000	-2.076586000
C	-1.668134000	-0.035255000	-0.302689000
C	-1.613592000	1.192006000	-1.004365000
C	-2.667892000	2.104526000	-0.879142000
C	-3.784422000	1.836749000	-0.086473000
C	-3.843684000	0.598899000	0.556628000
C	-2.816966000	-0.348503000	0.457343000
C	-0.452911000	1.581536000	-1.899464000
C	-4.891032000	2.851052000	0.073367000
C	-3.003298000	-1.664086000	1.179616000
H	2.567065000	2.209456000	2.388333000
H	4.696353000	0.922425000	-1.092745000
H	0.024502000	-0.230199000	2.371051000
H	0.601370000	1.299001000	3.040292000
H	-0.503772000	1.291831000	1.660300000
H	4.718867000	3.616677000	0.600633000
H	4.986343000	2.749606000	2.114077000
H	5.846819000	2.259422000	0.644180000
H	2.163594000	-0.527787000	-2.833589000
H	3.894322000	-0.631430000	-2.527646000
H	2.814320000	-1.867539000	-1.885490000
H	-2.615474000	3.045212000	-1.423735000
H	-4.722629000	0.354099000	1.149472000

H	0.400553000	1.950384000	-1.322675000
H	-0.090380000	0.743458000	-2.509347000
H	-0.753683000	2.366625000	-2.598672000
H	-4.716916000	3.485069000	0.951808000
H	-4.959654000	3.511416000	-0.796458000
H	-5.862508000	2.366255000	0.210903000
H	-4.047603000	-1.792586000	1.477201000
H	-2.727092000	-2.521055000	0.558277000
H	-2.386169000	-1.720984000	2.080655000
Sb	0.026438000	-1.375632000	-0.641147000
Cl	0.131103000	-2.746369000	1.350462000

2-Sb (g)

Total energy including ZPVE: -2053.614686 a. u.

Total electronic and thermal enthalpies: -2053.577602 a. u.

C	2.431759000	0.209354000	-0.050708000
C	3.146396000	-0.533447000	0.917610000
C	4.218136000	0.075005000	1.584729000
C	4.614703000	1.386116000	1.320093000
C	3.912344000	2.096276000	0.345251000
C	2.834135000	1.533764000	-0.348138000
C	2.837637000	-1.969899000	1.280871000
C	5.749928000	2.025652000	2.083347000
C	2.146550000	2.385291000	-1.398419000
C	-0.546456000	-1.495448000	0.257147000
C	-0.737085000	-0.986809000	1.568466000
C	-1.776884000	-1.500089000	2.356934000
C	-2.641277000	-2.499607000	1.903693000
C	-2.445927000	-2.984735000	0.611618000
C	-1.421238000	-2.503071000	-0.216962000
C	0.117584000	0.097480000	2.191118000
C	-3.732670000	-3.047020000	2.791506000
C	-1.317164000	-3.107243000	-1.601807000
C	-2.914124000	3.262051000	-1.223443000
C	-2.106225000	4.535317000	-0.935429000
C	-2.624699000	2.209156000	1.517745000

C	-4.010250000	2.770358000	1.866703000
C	-3.453573000	0.436167000	-0.639982000
C	-3.377487000	-0.033469000	-2.098731000
H	4.759450000	-0.499587000	2.334120000
H	4.212118000	3.116412000	0.113568000
H	3.367273000	-2.656356000	0.614262000
H	3.153077000	-2.180566000	2.307649000
H	1.777241000	-2.211304000	1.193809000
H	5.383631000	2.522489000	2.990872000
H	6.491028000	1.283562000	2.396136000
H	6.260602000	2.783990000	1.481627000
H	1.082696000	2.515119000	-1.180736000
H	2.608636000	3.375445000	-1.451561000
H	2.226226000	1.938333000	-2.396770000
H	-1.913901000	-1.102764000	3.361285000
H	-3.112622000	-3.754296000	0.227644000
H	1.100649000	-0.282046000	2.477728000
H	0.278394000	0.933745000	1.510305000
H	-0.359039000	0.481329000	3.098446000
H	-3.353847000	-3.861688000	3.421174000
H	-4.128472000	-2.277677000	3.462428000
H	-4.564240000	-3.449362000	2.204801000
H	-2.243071000	-3.625292000	-1.867725000
H	-1.127131000	-2.356434000	-2.375721000
H	-0.492239000	-3.822333000	-1.660251000
H	-3.982695000	3.410191000	-1.028883000
H	-2.814690000	2.977235000	-2.276591000
H	-1.040040000	4.361921000	-1.105734000
H	-2.428758000	5.353239000	-1.586305000
H	-2.232484000	4.865778000	0.101052000
H	-1.831417000	2.903166000	1.815238000
H	-2.437856000	1.272207000	2.051865000
H	-4.812860000	2.084935000	1.576706000
H	-4.092426000	2.929587000	2.946142000
H	-4.195388000	3.731949000	1.378182000
H	-4.472717000	0.747622000	-0.380869000
H	-3.178914000	-0.377899000	0.037914000
H	-3.975958000	-0.938655000	-2.235278000
H	-3.754614000	0.725174000	-2.792036000
H	-2.348550000	-0.267891000	-2.381978000
O	-0.855497000	1.535054000	-0.534624000

P	-2.321932000	1.822523000	-0.251574000
Sb	0.783697000	-0.583427000	-1.240393000
Cl	2.027801000	-2.628217000	-1.857125000

1-Bi (g)

Total energy including ZPVE: -1373.841012 a. u.

Total electronic and thermal enthalpies: -1373.816169 a. u.

C	1.655074000	0.212239000	0.100344000
C	1.605381000	0.985842000	1.280975000
C	2.658875000	1.870268000	1.548801000
C	3.749372000	2.016719000	0.688853000
C	3.778875000	1.240221000	-0.471041000
C	2.751802000	0.339945000	-0.779314000
C	0.469071000	0.905981000	2.275570000
C	4.849090000	3.005764000	0.992588000
C	2.862499000	-0.457291000	-2.065309000
C	-1.725931000	0.172720000	-0.201673000
C	-1.715986000	1.291402000	-1.063460000
C	-2.764991000	2.217262000	-1.001089000
C	-3.827143000	2.065249000	-0.108896000
C	-3.831285000	0.938156000	0.715985000
C	-2.806445000	-0.016810000	0.685322000
C	-0.602933000	1.543135000	-2.062278000
C	-4.930011000	3.093076000	-0.025028000
C	-2.904490000	-1.199823000	1.620705000
H	2.624225000	2.461571000	2.461543000
H	4.622597000	1.333456000	-1.151819000
H	0.326934000	-0.116142000	2.636823000
H	0.666043000	1.544747000	3.140673000
H	-0.475204000	1.227957000	1.827024000
H	4.595443000	4.003505000	0.612740000
H	5.014397000	3.101681000	2.070147000
H	5.794665000	2.710457000	0.527895000
H	2.056293000	-0.216897000	-2.770231000
H	3.803937000	-0.241894000	-2.577670000
H	2.834356000	-1.538425000	-1.885790000

H	-2.750973000	3.075077000	-1.670621000
H	-4.661160000	0.790770000	1.404260000
H	0.325848000	1.845089000	-1.567308000
H	-0.378389000	0.655671000	-2.671301000
H	-0.879723000	2.333062000	-2.765517000
H	-4.712682000	3.838852000	0.749906000
H	-5.050981000	3.630976000	-0.970217000
H	-5.889246000	2.631605000	0.229476000
H	-3.883611000	-1.230182000	2.106403000
H	-2.760373000	-2.151254000	1.099923000
H	-2.140091000	-1.156918000	2.401819000
Bi	0.031923000	-1.265454000	-0.517905000
Cl	0.155479000	-2.637908000	1.585975000

2-Bi (g)

Total energy including ZPVE: -2027.991576 a. u.

Total electronic and thermal enthalpies: -2027.953838 a. u.

C	-2.440724000	-0.224706000	0.163994000
C	-3.160440000	0.754934000	0.882675000
C	-4.268945000	0.356179000	1.642376000
C	-4.690781000	-0.973055000	1.705678000
C	-3.976002000	-1.922215000	0.973370000
C	-2.861323000	-1.572109000	0.200795000
C	-2.808793000	2.226057000	0.870227000
C	-5.867308000	-1.374406000	2.563444000
C	-2.149072000	-2.671198000	-0.565103000
C	0.674826000	1.509518000	0.217297000
C	0.793436000	1.268427000	1.607032000
C	1.799857000	1.926045000	2.331319000
C	2.693470000	2.815923000	1.731134000
C	2.567449000	3.035734000	0.358988000
C	1.581583000	2.397385000	-0.406378000
C	-0.103374000	0.322047000	2.375260000
C	3.745591000	3.531558000	2.544107000
C	1.563183000	2.671929000	-1.895648000
C	2.993398000	-2.844282000	1.523844000

C	2.727190000	-2.033309000	2.800032000
C	3.462068000	-0.477607000	-0.159352000
C	4.982931000	-0.679643000	-0.124975000
C	2.913873000	-3.082632000	-1.395525000
C	2.021726000	-4.328395000	-1.496481000
H	-4.819380000	1.112091000	2.199514000
H	-4.292967000	-2.963077000	1.001180000
H	-3.181438000	2.704776000	-0.039516000
H	-3.249062000	2.735601000	1.732643000
H	-1.729763000	2.397241000	0.889309000
H	-5.551209000	-1.584461000	3.593286000
H	-6.617972000	-0.579221000	2.610995000
H	-6.352927000	-2.277782000	2.181468000
H	-1.098981000	-2.756975000	-0.268517000
H	-2.629305000	-3.638359000	-0.390518000
H	-2.175591000	-2.492945000	-1.647840000
H	1.886101000	1.732458000	3.399046000
H	3.261357000	3.713080000	-0.135188000
H	-1.111799000	0.725505000	2.490997000
H	-0.197388000	-0.642223000	1.872749000
H	0.297438000	0.148834000	3.378486000
H	3.362373000	4.484570000	2.929654000
H	4.060589000	2.936468000	3.407250000
H	4.632305000	3.758498000	1.943706000
H	2.412042000	3.296241000	-2.188223000
H	1.624732000	1.746657000	-2.483917000
H	0.642927000	3.174512000	-2.203934000
H	4.058854000	-3.078734000	1.413948000
H	2.457135000	-3.799103000	1.557281000
H	1.659247000	-1.840326000	2.918849000
H	3.077228000	-2.581027000	3.679938000
H	3.238403000	-1.065674000	2.780416000
H	3.140423000	0.199875000	0.636364000
H	3.150909000	-0.001809000	-1.095528000
H	5.334201000	-1.336049000	-0.927484000
H	5.485138000	0.284777000	-0.244718000
H	5.314228000	-1.103356000	0.828385000
H	3.970953000	-3.354299000	-1.294238000
H	2.823918000	-2.474408000	-2.303691000
H	2.275181000	-4.910701000	-2.387071000
H	2.142948000	-4.982488000	-0.626988000

H	0.968119000	-4.043296000	-1.558540000
O	0.943822000	-1.700239000	0.005818000
P	2.439301000	-1.987641000	-0.000150000
Bi	-0.649022000	0.234737000	-1.175375000
Cl	-1.864892000	2.146790000	-2.401551000

$[(Mesityl)_2Sb]^+$ (g)

Total energy including ZPVE: -938.982771 a. u.

Total electronic and thermal enthalpies: -938.959663 a. u.

C	1.651347000	-0.203672000	0.105154000
C	1.683098000	0.955288000	0.944383000
C	2.867360000	1.677252000	1.022207000
C	4.023177000	1.317053000	0.302371000
C	3.978312000	0.174238000	-0.501423000
C	2.822767000	-0.599205000	-0.608778000
C	0.510043000	1.420323000	1.783004000
C	5.276105000	2.136706000	0.430688000
C	2.841842000	-1.784696000	-1.546956000
C	-1.651415000	-0.204076000	-0.105198000
C	-1.683814000	0.954079000	-0.945481000
C	-2.868188000	1.675809000	-1.023246000
C	-4.023531000	1.316138000	-0.302304000
C	-3.978041000	0.174067000	0.502432000
C	-2.822268000	-0.599120000	0.609792000
C	-0.511284000	1.418169000	-1.785366000
C	-5.276287000	2.136149000	-0.430091000
C	-2.840527000	-1.783746000	1.549052000
H	2.911770000	2.546083000	1.673923000
H	4.863375000	-0.116184000	-1.060637000
H	0.031185000	0.601026000	2.328097000
H	0.841779000	2.148578000	2.525995000
H	-0.263368000	1.897492000	1.175069000
H	5.062149000	3.203146000	0.303910000
H	5.707266000	2.015780000	1.432054000
H	6.033212000	1.844023000	-0.299761000
H	2.459360000	-1.511686000	-2.537414000

H	3.858457000	-2.160488000	-1.683759000
H	2.237049000	-2.626600000	-1.184409000
H	-2.913164000	2.543971000	-1.675820000
H	-4.862733000	-0.116032000	1.062396000
H	0.263247000	1.894640000	-1.178330000
H	-0.033815000	0.598400000	-2.331026000
H	-0.843186000	2.146674000	-2.528034000
H	-5.063048000	3.201670000	-0.294197000
H	-5.702960000	2.022977000	-1.434234000
H	-6.036408000	1.837974000	0.294963000
H	-3.856898000	-2.159993000	1.686429000
H	-2.235310000	-2.625647000	1.187157000
H	-2.457957000	-1.509620000	2.539169000
Sb	0.000153000	-1.505112000	-0.000059000

$[(Mesityl)_2Sb(OPEt_3)]^+$ (g)

Total energy including ZPVE: -1593.184245 a. u.

Total electronic and thermal enthalpies: -1593.148608 a. u.

C	-2.333626000	-0.056607000	-0.360798000
C	-3.038886000	1.168251000	-0.326302000
C	-4.301521000	1.202190000	0.271200000
C	-4.890631000	0.059549000	0.822965000
C	-4.196526000	-1.148558000	0.725142000
C	-2.932345000	-1.236384000	0.129960000
C	-2.483988000	2.451114000	-0.911961000
C	-6.237827000	0.133433000	1.497010000
C	-2.276402000	-2.598532000	0.047622000
C	0.622174000	1.535409000	-0.324804000
C	0.561873000	1.750597000	1.074837000
C	1.432429000	2.686986000	1.646443000
C	2.347019000	3.422865000	0.886427000
C	2.373784000	3.210085000	-0.494725000
C	1.525122000	2.286999000	-1.115671000
C	-0.406159000	1.039260000	1.997479000
C	3.248946000	4.444421000	1.532084000
C	1.605465000	2.147151000	-2.624907000

C	1.879986000	-3.157076000	1.604185000
C	1.395695000	-2.552297000	2.931766000
C	3.079536000	-0.593888000	0.692227000
C	4.492064000	-1.057483000	1.084171000
C	2.563531000	-2.760210000	-1.260532000
C	1.655610000	-3.891345000	-1.769883000
H	-4.846621000	2.142920000	0.294552000
H	-4.658165000	-2.055306000	1.108978000
H	-1.995789000	2.296335000	-1.883694000
H	-3.284226000	3.175253000	-1.082706000
H	-1.746237000	2.917029000	-0.251008000
H	-6.129434000	0.442706000	2.543736000
H	-6.889795000	0.863750000	1.009039000
H	-6.744435000	-0.835434000	1.492020000
H	-1.540932000	-2.741197000	0.845220000
H	-3.024773000	-3.390155000	0.132574000
H	-1.750306000	-2.749039000	-0.902230000
H	1.390605000	2.851133000	2.720821000
H	3.068891000	3.781986000	-1.104603000
H	-1.419958000	1.435484000	1.885040000
H	-0.465644000	-0.031995000	1.799956000
H	-0.111821000	1.178204000	3.040964000
H	2.762620000	5.427120000	1.551779000
H	3.484228000	4.177863000	2.566360000
H	4.187449000	4.557703000	0.982052000
H	2.355361000	2.825797000	-3.037821000
H	1.878725000	1.133859000	-2.942652000
H	0.652853000	2.392270000	-3.108690000
H	2.880008000	-3.594861000	1.701741000
H	1.208776000	-3.955808000	1.271525000
H	0.400008000	-2.114237000	2.826200000
H	1.343679000	-3.332826000	3.694475000
H	2.075302000	-1.776263000	3.296028000
H	2.600531000	-0.038142000	1.503993000
H	3.105395000	0.096517000	-0.157588000
H	4.993458000	-1.593123000	0.272795000
H	5.103123000	-0.184153000	1.324880000
H	4.480647000	-1.703121000	1.967088000
H	3.573984000	-3.125986000	-1.045448000
H	2.667144000	-1.971637000	-2.016038000
H	2.052787000	-4.289048000	-2.706740000

H	1.599463000	-4.718329000	-1.056606000
H	0.639937000	-3.533455000	-1.959381000
O	0.472766000	-1.440082000	0.039736000
P	1.940503000	-1.945868000	0.247857000
Sb	-0.409773000	-0.081739000	-1.316391000

$[(Mesityl)_2Bi]^+$ (g)

Total energy including ZPVE: -913.357898 a. u.

Total electronic and thermal enthalpies: -913.334537 a. u.

C	1.713647000	0.041227000	0.119849000
C	1.725072000	1.188828000	0.966478000
C	2.894732000	1.937356000	1.040479000
C	4.050993000	1.606984000	0.308186000
C	4.020611000	0.472595000	-0.507601000
C	2.877827000	-0.322575000	-0.612513000
C	0.541954000	1.619914000	1.808623000
C	5.288737000	2.451425000	0.432475000
C	2.907263000	-1.496273000	-1.565943000
C	-1.713576000	0.041487000	-0.119832000
C	-1.724633000	1.189496000	-0.965892000
C	-2.894183000	1.938261000	-1.039808000
C	-4.050665000	1.607678000	-0.308037000
C	-4.020615000	0.472912000	0.507312000
C	-2.878027000	-0.322486000	0.612096000
C	-0.541231000	1.621020000	-1.807412000
C	-5.288836000	2.451383000	-0.433046000
C	-2.907877000	-1.496589000	1.565025000
H	2.924990000	2.802891000	1.697560000
H	4.905627000	0.205634000	-1.078769000
H	0.115017000	0.792509000	2.385487000
H	0.843610000	2.385363000	2.526696000
H	-0.263124000	2.037284000	1.197763000
H	5.055239000	3.512316000	0.293372000
H	5.720496000	2.349514000	1.435481000
H	6.052681000	2.166437000	-0.293999000
H	2.500642000	-1.222289000	-2.546539000

H	3.928906000	-1.848297000	-1.726953000
H	2.332928000	-2.358760000	-1.200033000
H	-2.924074000	2.804204000	-1.696362000
H	-4.905773000	0.205902000	1.078244000
H	0.263309000	2.038777000	-1.196102000
H	-0.113579000	0.793794000	-2.383978000
H	-0.842825000	2.386312000	-2.525679000
H	-5.054118000	3.513849000	-0.309595000
H	-5.728708000	2.336381000	-1.431172000
H	-6.047213000	2.175744000	0.302843000
H	-3.929614000	-1.848556000	1.725562000
H	-2.333538000	-2.358995000	1.198952000
H	-2.501533000	-1.223052000	2.545861000
Bi	-0.000078000	-1.345335000	-0.000015000

$[(Mesityl)_2Bi(OPEt_3)]^+$ (g)

Total energy including ZPVE: -1567.557333 a. u.

Total electronic and thermal enthalpies: -1567.521252 a. u.

C	-2.389582000	-0.069736000	-0.170259000
C	-3.095314000	1.151460000	-0.114361000
C	-4.334011000	1.180198000	0.532831000
C	-4.891371000	0.036291000	1.115291000
C	-4.189547000	-1.166594000	1.005900000
C	-2.948119000	-1.248165000	0.362520000
C	-2.564360000	2.431673000	-0.726762000
C	-6.212716000	0.105232000	1.839627000
C	-2.263917000	-2.595702000	0.280701000
C	0.663659000	1.591212000	-0.209782000
C	0.623153000	1.782727000	1.190975000
C	1.506612000	2.708224000	1.763220000
C	2.411701000	3.451819000	0.999112000
C	2.416268000	3.259427000	-0.385663000
C	1.555145000	2.346564000	-1.004832000
C	-0.335492000	1.057164000	2.111343000
C	3.327442000	4.460987000	1.645477000
C	1.611920000	2.214226000	-2.515477000

C	2.113896000	-2.956250000	1.915988000
C	1.703844000	-2.185218000	3.180456000
C	3.205670000	-0.524824000	0.610326000
C	4.647028000	-0.908731000	0.982209000
C	2.661489000	-2.947641000	-0.997376000
C	1.740711000	-4.135102000	-1.321603000
H	-4.885127000	2.116919000	0.572899000
H	-4.624696000	-2.072229000	1.422026000
H	-2.184392000	2.283591000	-1.747408000
H	-3.352981000	3.184110000	-0.801926000
H	-1.748818000	2.859936000	-0.135119000
H	-6.068833000	0.435342000	2.875645000
H	-6.892886000	0.817818000	1.363990000
H	-6.705984000	-0.869970000	1.871463000
H	-1.453000000	-2.680700000	1.010093000
H	-2.975190000	-3.403783000	0.467557000
H	-1.823723000	-2.775526000	-0.708036000
H	1.481908000	2.856849000	2.840488000
H	3.104215000	3.837357000	-0.998250000
H	-1.349198000	1.459290000	2.020463000
H	-0.400319000	-0.009208000	1.889396000
H	-0.027465000	1.170791000	3.153985000
H	2.844588000	5.444558000	1.690249000
H	3.580345000	4.176669000	2.670870000
H	4.256671000	4.580939000	1.081238000
H	2.339877000	2.908213000	-2.942032000
H	1.905524000	1.207641000	-2.840132000
H	0.646695000	2.442919000	-2.983152000
H	3.125606000	-3.368087000	2.007407000
H	1.438196000	-3.799195000	1.736647000
H	0.693746000	-1.779533000	3.086179000
H	1.720478000	-2.855875000	4.042908000
H	2.387290000	-1.357024000	3.390209000
H	2.758683000	0.127784000	1.366500000
H	3.174730000	0.047595000	-0.322877000
H	5.118368000	-1.539791000	0.223146000
H	5.249461000	-0.001544000	1.073205000
H	4.695409000	-1.431606000	1.941846000
H	3.679415000	-3.283011000	-0.769117000
H	2.738010000	-2.267265000	-1.854686000
H	2.100368000	-4.650707000	-2.215215000

H	1.717792000	-4.863365000	-0.506048000
H	0.715898000	-3.803496000	-1.510107000
O	0.594279000	-1.497645000	0.176883000
P	2.072929000	-1.939451000	0.405735000
Bi	-0.417030000	-0.100108000	-1.247043000

3-Sb (g)

Total energy including ZPVE: -1900.645737 a. u.

Total electronic and thermal enthalpies: -1900.614489 a. u.

C	0.781681000	-1.477231000	0.241771000
C	0.815222000	-1.705243000	-1.153933000
C	1.561157000	-2.787651000	-1.639155000
C	2.269419000	-3.646552000	-0.797007000
C	2.223009000	-3.403406000	0.577820000
C	1.493626000	-2.336827000	1.111343000
C	0.107489000	-0.832489000	-2.167005000
C	3.035270000	-4.822983000	-1.351777000
C	1.483969000	-2.164625000	2.619223000
C	-2.241677000	-0.016820000	0.331552000
C	-2.868009000	-1.276331000	0.182247000
C	-4.159995000	-1.332423000	-0.350505000
C	-4.856407000	-0.182083000	-0.730408000
C	-4.241689000	1.053355000	-0.523955000
C	-2.952469000	1.163849000	0.012242000
C	-2.212775000	-2.583819000	0.579894000
C	-6.231762000	-0.274654000	-1.345208000
C	-2.395408000	2.557203000	0.220729000
C	2.878361000	1.920055000	-0.641544000
H	1.588191000	-2.961211000	-2.712819000
H	2.767632000	-4.061083000	1.251747000
H	0.692363000	0.067614000	-2.372773000
H	-0.027989000	-1.372966000	-3.107794000
H	-0.873791000	-0.502748000	-1.820489000
H	2.400697000	-5.717090000	-1.394389000
H	3.390505000	-4.626907000	-2.367761000
H	3.900567000	-5.067710000	-0.728340000

H	0.481210000	-2.299427000	3.044756000
H	2.130907000	-2.904797000	3.097197000
H	1.839786000	-1.175101000	2.927332000
H	-4.639641000	-2.302583000	-0.462557000
H	-4.782894000	1.963160000	-0.774850000
H	-1.493525000	-2.922949000	-0.171079000
H	-1.669035000	-2.512080000	1.528559000
H	-2.966635000	-3.366248000	0.702797000
H	-6.164646000	-0.371948000	-2.435990000
H	-6.779880000	-1.146093000	-0.974158000
H	-6.826874000	0.618882000	-1.134256000
H	-3.208572000	3.282091000	0.313314000
H	-1.789271000	2.637467000	1.130319000
H	-1.760403000	2.868009000	-0.613667000
O	0.328419000	1.474752000	-0.342768000
O	1.404401000	3.057008000	1.280073000
O	0.956355000	3.728544000	-1.132596000
S	1.269410000	2.714592000	-0.135598000
F	3.134848000	0.889416000	0.176592000
F	3.867751000	2.808392000	-0.556392000
F	2.792058000	1.468568000	-1.896371000
Sb	-0.257228000	0.171617000	1.181066000

3-Bi (g)

Total energy including ZPVE: -1875.018991 a. u.

Total electronic and thermal enthalpies: -1874.987215 a. u.

C	0.823831000	1.518548000	-0.158559000
C	0.886065000	1.731921000	1.235512000
C	1.657052000	2.800400000	1.713713000
C	2.361176000	3.654683000	0.862823000
C	2.283633000	3.423257000	-0.512883000
C	1.527572000	2.370201000	-1.037481000
C	0.180146000	0.856890000	2.247176000
C	3.156242000	4.815258000	1.410479000
C	1.482359000	2.197874000	-2.544501000
C	-2.322290000	0.018018000	-0.144874000

C	-2.923349000	1.283248000	0.037147000
C	-4.192957000	1.352351000	0.622091000
C	-4.885758000	0.207767000	1.024914000
C	-4.291603000	-1.034276000	0.794629000
C	-3.025793000	-1.155886000	0.207008000
C	-2.260629000	2.582615000	-0.373594000
C	-6.235078000	0.312227000	1.693549000
C	-2.477760000	-2.549111000	-0.022207000
C	2.926569000	-1.827409000	0.997796000
H	1.708518000	2.965735000	2.787861000
H	2.824210000	4.077866000	-1.193316000
H	0.729909000	-0.074109000	2.405253000
H	0.099305000	1.370460000	3.209092000
H	-0.826656000	0.582474000	1.924359000
H	2.538372000	5.720121000	1.469067000
H	3.525814000	4.607333000	2.418983000
H	4.014994000	5.048592000	0.773677000
H	0.468897000	2.331182000	-2.946447000
H	2.113815000	2.938731000	-3.041684000
H	1.839390000	1.210172000	-2.860423000
H	-4.656543000	2.327260000	0.758638000
H	-4.830497000	-1.938479000	1.069701000
H	-1.485510000	2.884457000	0.336603000
H	-1.780020000	2.518371000	-1.357017000
H	-2.997139000	3.388621000	-0.432496000
H	-6.125105000	0.392685000	2.782224000
H	-6.783575000	1.196844000	1.355787000
H	-6.851643000	-0.569242000	1.493396000
H	-3.277419000	-3.292270000	0.033351000
H	-2.013486000	-2.653350000	-1.010858000
H	-1.715137000	-2.812866000	0.715196000
O	0.383207000	-1.590819000	0.445366000
O	1.823741000	-2.680463000	-1.276982000
O	1.217545000	-3.887665000	0.877931000
S	1.486896000	-2.653967000	0.151144000
F	3.148727000	-0.633378000	0.433355000
F	4.017368000	-2.584151000	0.874465000
F	2.655978000	-1.649885000	2.296378000
Bi	-0.290627000	-0.193136000	-1.135349000

4-Sb (g)

Total energy including ZPVE: -2554.799744 a. u.

Total electronic and thermal enthalpies: -2554.755610 a. u.

C	1.308856000	1.514323000	0.466868000
C	2.014488000	1.359458000	1.683198000
C	2.745797000	2.445559000	2.182690000
C	2.817241000	3.669074000	1.516355000
C	2.140586000	3.792117000	0.301600000
C	1.395518000	2.738731000	-0.239408000
C	2.067109000	0.073296000	2.479817000
C	3.585393000	4.830158000	2.100511000
C	0.717901000	2.964648000	-1.577186000
C	-1.003436000	-0.970919000	1.050777000
C	-1.588126000	-0.251111000	2.123074000
C	-2.468153000	-0.913909000	2.987463000
C	-2.815337000	-2.256496000	2.818378000
C	-2.252832000	-2.943131000	1.742686000
C	-1.347387000	-2.331369000	0.862569000
C	-1.335376000	1.218351000	2.385400000
C	-3.754750000	-2.943682000	3.779987000
C	-0.768786000	-3.193594000	-0.242259000
C	4.237014000	-1.186472000	-0.748329000
C	-4.237143000	2.172524000	-1.975363000
C	-4.476780000	3.312436000	-0.974423000
C	-4.260757000	0.078792000	0.109213000
C	-5.728999000	-0.220536000	-0.224321000
C	-3.132297000	-0.502425000	-2.524003000
C	-2.329815000	-0.082439000	-3.763972000
H	3.282134000	2.323664000	3.121729000
H	2.198805000	4.731004000	-0.245174000
H	2.878076000	-0.562655000	2.115764000
H	2.250882000	0.287130000	3.537073000
H	1.153044000	-0.515830000	2.403799000
H	2.941443000	5.442545000	2.744483000
H	4.425603000	4.487774000	2.712315000
H	3.978830000	5.485295000	1.317074000
H	-0.370488000	2.897034000	-1.496982000
H	0.972082000	3.950984000	-1.974986000

H	1.036539000	2.224204000	-2.321034000
H	-2.911334000	-0.355651000	3.809913000
H	-2.516651000	-3.986590000	1.582393000
H	-0.349129000	1.386444000	2.825323000
H	-1.386003000	1.807494000	1.468717000
H	-2.078347000	1.610900000	3.086509000
H	-3.206783000	-3.344615000	4.641640000
H	-4.508117000	-2.251587000	4.169776000
H	-4.273286000	-3.782597000	3.305758000
H	-1.411304000	-4.057383000	-0.435536000
H	-0.647199000	-2.656384000	-1.189430000
H	0.223125000	-3.565852000	0.031203000
H	-5.180057000	1.770538000	-2.363203000
H	-3.660236000	2.531918000	-2.834207000
H	-3.528048000	3.675628000	-0.570045000
H	-4.986051000	4.149270000	-1.460614000
H	-5.099354000	2.985895000	-0.135022000
H	-4.180053000	0.774090000	0.950506000
H	-3.736124000	-0.829351000	0.421293000
H	-5.825972000	-0.916591000	-1.063586000
H	-6.216798000	-0.683211000	0.638509000
H	-6.288205000	0.687098000	-0.471752000
H	-4.147750000	-0.813870000	-2.795878000
H	-2.658610000	-1.358833000	-2.029723000
H	-2.239141000	-0.924002000	-4.456255000
H	-2.814761000	0.739029000	-4.300636000
H	-1.320882000	0.234694000	-3.488712000
O	1.775241000	-1.503064000	0.040219000
O	2.268918000	-1.946336000	-2.374604000
O	3.012768000	-3.559386000	-0.566680000
O	-1.904181000	1.324437000	-0.773576000
P	-3.264070000	0.803940000	-1.245151000
S	2.693802000	-2.199626000	-0.993204000
F	3.977977000	0.100790000	-1.020461000
F	5.203760000	-1.618370000	-1.562304000
F	4.659028000	-1.280961000	0.519896000
Sb	0.217488000	-0.078850000	-0.522500000

4-Bi (g)

Total energy including ZPVE: -2529.177736 a. u.

Total electronic and thermal enthalpies: -2529.133170 a. u.

C	1.336333000	1.458410000	0.601843000
C	2.024645000	1.198566000	1.806538000
C	2.757225000	2.236553000	2.399668000
C	2.841435000	3.509203000	1.833854000
C	2.174155000	3.736160000	0.628170000
C	1.428722000	2.732804000	-0.000909000
C	2.052514000	-0.151496000	2.489200000
C	3.611830000	4.614660000	2.515554000
C	0.750358000	3.061890000	-1.316840000
C	-1.080147000	-1.124495000	1.052396000
C	-1.709012000	-0.415093000	2.102114000
C	-2.682207000	-1.064521000	2.876047000
C	-3.047330000	-2.394647000	2.652189000
C	-2.407846000	-3.081860000	1.619138000
C	-1.433874000	-2.472938000	0.815845000
C	-1.382507000	1.020977000	2.450948000
C	-4.078512000	-3.075257000	3.520212000
C	-0.815689000	-3.298436000	-0.294948000
C	4.379798000	-1.151013000	-0.565875000
C	-4.562440000	2.207667000	-0.538350000
C	-4.628922000	2.188459000	0.995822000
C	-3.934524000	-0.663935000	-0.739639000
C	-5.384253000	-1.004576000	-1.111634000
C	-3.491984000	1.103872000	-3.044456000
C	-2.902949000	2.402690000	-3.614809000
H	3.284156000	2.036429000	3.330714000
H	2.239854000	4.716978000	0.161247000
H	2.847091000	-0.774158000	2.070558000
H	2.241057000	-0.035879000	3.560879000
H	1.122865000	-0.709134000	2.364095000
H	2.964119000	5.186170000	3.192566000
H	4.437704000	4.217686000	3.113696000
H	4.026356000	5.321009000	1.789489000
H	-0.337717000	2.970603000	-1.243573000
H	0.984664000	4.083019000	-1.630089000

H	1.086545000	2.395660000	-2.121871000
H	-3.166997000	-0.512424000	3.679203000
H	-2.678281000	-4.117943000	1.425150000
H	-0.402743000	1.100128000	2.929340000
H	-1.358653000	1.661427000	1.567873000
H	-2.122610000	1.423531000	3.149121000
H	-3.605679000	-3.555697000	4.385738000
H	-4.813055000	-2.361750000	3.906953000
H	-4.615337000	-3.854903000	2.970670000
H	-1.306065000	-4.271961000	-0.377886000
H	-0.906841000	-2.809100000	-1.274141000
H	0.251459000	-3.464990000	-0.126899000
H	-5.541491000	1.996564000	-0.984256000
H	-4.251786000	3.194710000	-0.897854000
H	-3.655634000	2.427033000	1.429366000
H	-5.353478000	2.925800000	1.352951000
H	-4.932062000	1.208124000	1.376482000
H	-3.774407000	-0.752176000	0.338760000
H	-3.235548000	-1.370369000	-1.199845000
H	-5.562461000	-0.945251000	-2.189887000
H	-5.612636000	-2.026562000	-0.796278000
H	-6.097840000	-0.341603000	-0.612396000
H	-4.542668000	0.980811000	-3.331214000
H	-2.948472000	0.234803000	-3.434561000
H	-2.931260000	2.385182000	-4.707824000
H	-3.464679000	3.281388000	-3.282095000
H	-1.863402000	2.527350000	-3.300592000
O	1.860714000	-1.659851000	-0.095040000
O	2.538582000	-1.360383000	-2.472294000
O	3.184654000	-3.453722000	-1.197392000
O	-1.938176000	1.314747000	-0.747174000
P	-3.360163000	1.006090000	-1.218569000
S	2.865479000	-2.028073000	-1.201522000
F	4.143798000	0.165916000	-0.483662000
F	5.410950000	-1.358058000	-1.390098000
F	4.701060000	-1.604516000	0.655221000
Bi	0.190281000	-0.120614000	-0.563990000

$OPEt_3$

Total energy including ZPVE: -654.124084 a. u.

Total electronic and thermal enthalpies: -654.111685 a. u.

C	0.499012000	-1.186048000	-0.868415000
C	1.763831000	-1.927091000	-0.415010000
C	1.132687000	1.228056000	0.678113000
C	1.671327000	1.930475000	-0.575703000
C	-1.556091000	0.826258000	-0.390605000
C	-2.776243000	-0.078789000	-0.609942000
H	0.676704000	-0.618219000	-1.789425000
H	-0.302822000	-1.901424000	-1.082323000
H	1.585051000	-2.450644000	0.528267000
H	2.073632000	-2.663348000	-1.162873000
H	2.600811000	-1.237083000	-0.263635000
H	1.942152000	0.729626000	1.222822000
H	0.697506000	1.952209000	1.376568000
H	0.878841000	2.445309000	-1.127834000
H	2.419836000	2.681036000	-0.303252000
H	2.151183000	1.223679000	-1.259883000
H	-1.208132000	1.259162000	-1.335993000
H	-1.817500000	1.661664000	0.269906000
H	-3.621152000	0.496553000	-1.000526000
H	-2.560361000	-0.877421000	-1.327157000
H	-3.079970000	-0.545699000	0.330717000
O	-0.550492000	-0.757390000	1.701154000
P	-0.162599000	-0.056897000	0.426985000

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