Electronic Supplementary Material (ESI) for Chemical Science.

Tris(benzoimidazol)amine (L) complexes of pnictogen(III) and pnictogen(V) cations and assessment of the $[LP]^{3+}/[LPF_2]^{3+}$ redox couple

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Supporting Information

Experimental

General Considerations

All air- and moisture-sensitive manipulations were carried out using standard vacuum line Schlenk techniques or in an MBraun Labmaster inert atmosphere dry-box containing an atmosphere of purified nitrogen. THF-d_8, CD_2Cl_2 and C_6D_6 were purchased from Sigma Aldrich. CD_2Cl_2 was dried over CaH_2 and distilled, THF-d_8 and C_6D_6 were distilled over potassium. All glassware was stored in a 170°C oven for several hours and was degassed prior to use. Solvents were distilled over the appropriate drying agent. Anhydrous grade MeCN was obtained from Sigma-Aldrich and used without distillation but stored over 3 Å molecular sieves. Solvents were additionally tested using a ketyl test to guarantee oxygen and moisture free conditions. TMSOTf (99%) was distilled under reduced pressure before use. $BIMH_3$[S1] and $BIMEt_3$[S2] were synthesized following literature procedures.

NMR tubes fitted with J-Young valves were charged and sealed inside the glovebox. ^1H NMR spectra were recorded on Bruker spectrometers operating at 300, 360 MHz, ^{13}C NMR at 76 MHz. ^{31}P NMR at 121.6 MHz, ^{19}F NMR at 282.5 MHz. All ^1H and ^{13}C NMR chemical shifts are reported relative to $SiMe_4$ using the ^1H (residual) and ^{13}C chemical shifts of the solvent as a secondary standard.

Infrared spectra were obtained on a Perkin Elmer Frontier instrument. Elemental analysis was performed at the University of Windsor Mass Spectrometry Service Laboratory using a Perkin Elmer 2400 combustion CHN analyser. All quantum chemical calculations were carried out using Gaussian 16. [S3]

Crystals for investigation were covered in Paratone®, mounted into a goniometer head, and then rapidly cooled under a stream of cold N_2 of the low-temperature apparatus (Oxford Cryostream) attached to the diffractometer. The data were then collected using the APEXII (Bruker AXS) software suite on a Bruker Photon 100 CMOS diffractometer using a graphite monochromator with MoK_α (λ = 0.71073 Å). For each sample, data were collected at low temperature. APEXII software was used for data reductions and SADABS (Bruker AXS) was used for absorption corrections (multi-scan; semi-empirical from equivalents). XPREP was used to determine the space group and the structures were solved and refined using the SHELX[S4] software suite as implemented in the WinGX[S5] or OLEX2[S6] program suites. Validation of the structures was conducted using PLATON and the structures have been deposited in the Cambridge Structural Database (CCDC 1578584-1578587, 1581022, 1581023).[S7]

Synthesis of P(BIM): A 100 mL Schlenk flask was charged with $BIMH_3$ (500 mg, 1.23 mmol) and NaH (90 mg, 3.74 mmol) in 30 mL THF at room temperature. After bubbling stops, the reaction was left to stir for 30 mins followed by the addition of PCl_3 (0.117 mL, 1.28 mmol) yielding in white precipitate. The reaction mixture was allowed to stir for 24 hours before solvent was removed under reduced pressure. DCM (30 mL) was added and the resulting suspension was filtered through celite® and washed with DCM (2 x 10 mL). Solvent from the filtrate was removed under reduced pressure to result in P(BIM) as a colourless solid, 0.367 g (69 %). Slow evaporation from THF or acetonitrile yields colourless crystals suitable for X-ray diffraction $C_{24}H_{18}N_7P \bullet THF$, **MW** = 507.53 g/mol, **MP** = 185 (dec.)**EA [calc.]:** C, 66.26; H, 5.16; N, 19.32 **EA [found.]:** C, 66.23; H, 5.04; N,18.87. **^{1}H NMR** (500 MHz, CD_2Cl_2) δ = 8.05 (d, 3H, $^3J_{HH}$ = 7 Hz), 7.65 (d, 3H, $^3J_{HH}$ = 7 Hz), 7.38 (t, 3H, $^3J_{HH}$ = 7 Hz), 7.31 (t, 3H, $^3J_{HH}$ = 7 Hz), 4.56 (s, 6H). **^{13}C{^{1}H} NMR** (125.76 MHz, CD_2Cl_2) δ = 155.07 (d, J_{CP} = 8.7 Hz), 144.75 (d, J_{CP} = 7.2

Hz), 138.12 (d, J_{CP} = 36.9 Hz), 124.31 (s), 124.18 (s), 120.19 (s), 111.87 (d, J_{CP} = 24.5 Hz), 51.16 (s). **^{31}P{^{1}H} NMR** (202.46 MHz, CD_2Cl_2) δ = 44.83 (s).

Synthesis of [P(BIMEt$_3$)][OTf]$_3$: To a rapidly stirred suspension of PCl_3 (1 mmol, 88 µL) and $BIMEt_3$ (1 mmol, 500 mg) in 8 mL of MeCN, AgOTf (3 mmol, 770 mg) were added, producing a cloudy mixture due to precipitation of AgCl. The mixture was then filtered and the clear solution was concentrated to half its volume, layered with 6 mL of diethyl ether and placed in the freezer at -35 °C. Colourless blocks were isolated from after 72 hours. Yield: 1024 mg (94 %) of the composition $C_{33}H_{33}F_9N_7O_9PS_3$ **MW** = 1093.0 g/mol, **MP** = 184 °C (brown) – 241 °C (black) (dec.) **EA [calc.]** $C_{33}H_{33}F_9N_7O_9PS_3$: C, 40.86; H, 3.43; N, 9.99 **EA [found.]:** C, 40.10; H, 3.89 ; N, 9.99 **^{1}H NMR** (300 MHz, MeCN-d3) δ = 8.68 (*pseudo-d* (broad), *J* = 8.59 Hz, 3H), 7.92 (*pseudo-d* (broad), *J* = 8.20 Hz, 3H), 7.84 (ddd, *J* = 1.2, 7.2, 8.4 Hz, 3H), 7.75 (ddd, *J* = 0.9, 7.4, 8.2 Hz, 3H). 5.38 (d, $J_{P,H}$ =0.7 Hz, 6H), 4.47 (quart, *J* = 7.4 Hz, 6H), 1.53 (t, *J* = 7.4 Hz, 9H). **^{19}F{^{1}H} NMR** (283 MHz, CD_3CN): δ = -79.6 (s). **^{13}C{^{1}H} NMR** (75.5 MHz CD_3CN): δ = 155.18 (d, *J* = 9.2 Hz, 1C), 134.67 (d, *J* = 40.6 Hz, 1C), 132.92 (d, *J* = 5.8 Hz, 1C), 128.26 (d, *J* = 1.9 Hz, 1C), 128.09 (d, *J* = 1.6 Hz, 1C), 114.39 (d, *J* = 27.8 Hz, 1C), 113.6 (s), 54.9 (s), 42.3 (s), 12.3 (s). **^{31}P{^{1}H} NMR** (121.4 MHz , CD_3CN): δ = 56.1 (s)

Synthesis of [AsCl(BIMEt$_3$)][OTf]$_2$: To a suspension of $AsCl_3$ (1 mmol, 83 µL) and $BIMEt_3$ (1 mmol, 500 mg) in 6 mL of MeCN, TMSOTf (5 mmol, 470 µL) was slowly added to yield a clear yellow solution. The solution was left at room temperature for 30 minutes. The mixture was then filtered over a glass filter and the light yellow solution was layered with 6 mL of diethyl ether and placed in the freezer at -35 °C. A crystalline colourless solid was isolated from the solution within 2 days. Yield: 310 mg (32 %) of the composition $C_{32}H_{33}ClF_6N_7O_6AsS_2 \cdot (MeCN)_2$, MW = 982.25 g/mol **MP** = 112 °C (dec.). **EA [calc.]** $C_{32}H_{33}ClF_6N_7O_6AsS_2$**:** C, 42.70; H, 3.70; N, 10.89. **EA [found.]:** C, 42.72; H, 3.95; N 10.79. **^{1}H NMR** (300 MHz, CD_3CN) δ = 8.29 (*pseudo-d* (broad), *J* = 7.1 Hz, 3H), 7.70 (*pseudo-d* (broad), *J* = 7.1 Hz, 3H), 7.6 – 7.4 (m, 6H), 5.35 (s, 6H), 4.31 (quart, *J* = 7.21 Hz, 6H), 1.38 (t, *J* = 7.21 Hz, 9H). **^{19}F{^{1}H} NMR** (283 MHz, CD_3CN): δ = -79.28 (s). **^{13}C{^{1}H} NMR** (75.5 MHz, CD_3CN): δ = 150.9 (s), 136.2 (s), 134.2 (s), 125.8 (s), 125.5 (s), 117.9 (s), 112.2 (s), 55.5 (s), 40.9 (s), 13.5 (s).

Synthesis of [As(BIMEt$_3$)][OTf]$_3$: To a suspension of $AsCl_3$ (0.2 mmol, 16.6 µL) and $BIMEt_3$ (0.2 mmol, 100 mg) in 3 mL of MeCN, TMSOTf (1 mmol, 200 µL) was slowly added to yield a clear yellow solution. The solution was left at room temperature for 30 minutes. AgOTf (0.375 mmol, 96 mg) was added, producing a cloudy yellow mixture due to precipitation of AgCl. The mixture was then filtered through Celite. The volatiles were removed under reduced pressure to yield a yellow oily precipitate, which was titurated with 1 mL of DCM and 4 mL of diethyl ether. The leftover colourless solid was dried under reduced pressure to isolate 148 mg of a colourless solid. Single crystals for X-ray diffraction analysis were grown from MeCN solutions layered with diethyl ether at -35 °C. Yield: 148 mg (68 %) of the composition $C_{33}H_{33}F_9N_7O_9AsS_3 \cdot MeCN_2$, MW = 1095.9 g/mol **MP** = 161 °C (dec.). **EA [calc.]** for $C_{33}H_{33}F_9N_7O_9AsS_3$: C, 39.10; H, 3.28; N, 9.67. **EA [found.]:** C, 38.80; H, 3.52; N 9.69. **^{1}H NMR** (300 MHz, CD_3CN) δ = 8.30 – 8.18 (*m,* 3H), 7.81 – 7.72 (*m,* 3H), 7.68 – 7.53 (*m,* 6H), 5.87 (s, 6H), 4.38 (quart, *J* = 7.32 Hz, 6H), 1.48 (t, *J* = 7.32 Hz, 9H). **^{19}F{^{1}H} NMR** (283 MHz, CD_3CN): δ = -79.3. **^{13}C{^{1}H} NMR** (75.5 MHz, CD_3CN): δ = 149.5 (s, C_{arom}), 134.7 (s, C_{arom}), 133.4 (s, C_{arom}), 126.3 (s, C_{arom}), 126.2 (s, C_{arom}), 116.0 (s, C_{arom}), 112.64 (s, C_{arom}), 61.2 (s, CH_2), 41.5 (s, CH_2), 13.0 (s, CH_3).

Synthesis of [SbF(BIMEt$_3$)][OTf]$_2$: To a solution of $SbF(OTf)_2$ (0.2 mmol, 88 mg) in 3 mL of MeCN, $BIMEt_3$ (0.2 mmol, 100 mg) was added as a solid. The solution was left to stir for 16 hours at room temperature, then the mixture was layered with 4 mL of diethyl ether and placed in the freezer at -

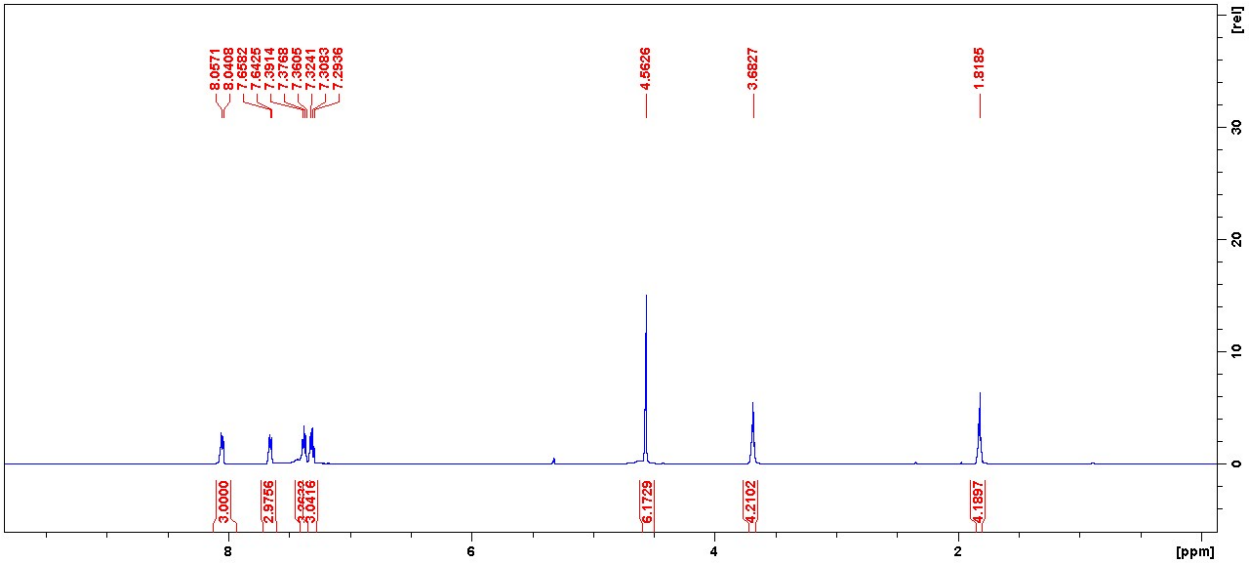
35 °C. Colourless crystals suitable for X-ray crystallography were isolated. Yield: 192 mg (92 %), $C_{32}H_{33}F_7N_7O_6S_2Sb\cdot(MeCN)_2$, MW = 1012.6 g/mol, MP = 183°C (grey) – 220 °C (black), **EA [calc.]** for $C_{32}H_{33}F_7N_7O_6S_2Sb$: C, 41.30; H, 3.57; N, 10.54; **EA [found.]**: C, 40.69; H, 3.56; N, 10.18; **^{1}H NMR** (300 MHz, CD_3CN) δ = 8.17 – 8.0 (*m,* 3H), 7.70 – 7.55 (*m,* 3H), 7.52 – 7.3 (*m,* 6H), 5.1 (s, 6H), 4.25 (quart, *J* = 7.32 Hz, 6H), 1.35 (t, *J* = 7.32 Hz, 9H). **^{19}F{^{1}H}** NMR (283 MHz, CD_3CN): δ = -79.25 (s). **^{13}C{^{1}H} NMR** (75.5 MHz, CD_3CN): δ = 151.0 (s, C_{arom}), 134.6 (s, C_{arom}), 126.0 (s, C_{arom}), 125.8 (s, C_{arom}), 116.0 (s, C_{arom}), 112.3 (s, C_{arom}), 58.6 (s, CH_2), 40.6 (s, CH_2), 13.2 (s, CH_3).

Synthesis of [Sb(BIMEt$_3$)][OTf]$_3$: To a solution of $SbFOTf_2$ (0.2 mmol, 88 mg) in 4 mL of MeCN, $BIMEt_3$ (0.2 mmol, 100 mg) was added. To the light yellow solution an excess TMSOTf (0.5 mmol, 100 µL) was added. The solution was left to stir for 30 minutes. ^{19}F NMR spectroscopy showed no presence of remaining fluoride bound antimony. The mixture was filtered and the clear yellow solution was layered with 2 mL of diethyl ether and was placed in the freezer at -25 °C for 16 hours. Colourless blocks suitable for X-ray crystallography were isolated by decantation of the solvent. The mother liquor was concentrated and layered with 8 mL of ether to isolate another crop of microcrystalline product. $C_{33}H_{33}F_9N_7O_9S_3Sb$, Yield: 188 mg (89 %) **MW** = 1060.6 g/mol. **MP** = 204 °C (melt and dec.). **EA [calc.]:** C, 37.37; H, 3.14; N, 9.24. **EA [found.]:** C, 37.71; H, 3.34; N, 9.23. **^{1}H NMR** (300 MHz, CD_3CN) δ = 8.27 – 8.17 (*m,* 3H), 7.75 – 7.65 (*m,* 3H), 7.44 – 7.55 (*m,* 6H), 5.45 (s, 6H), 4.28 (quart, *J* = 7.34 Hz, 6H), 1.38 (t, *J* = 7.34 Hz, 9H). **^{19}F{^{1}H} NMR** (283 MHz, CD_3CN): δ = -79.25 (s). **^{13}C{^{1}H} NMR** (75.5 MHz, CD_3CN): δ = 151.0 (s, C_{arom}), 134.6 (s, C_{arom}), 126.0 (s, C_{arom}), 125.8 (s, C_{arom}), 116.0 (s, C_{arom}), 112.3 (s, C_{arom}), 58.6 (s, CH_2), 40.6 (s, CH_2), 13.2 (s, CH_3).

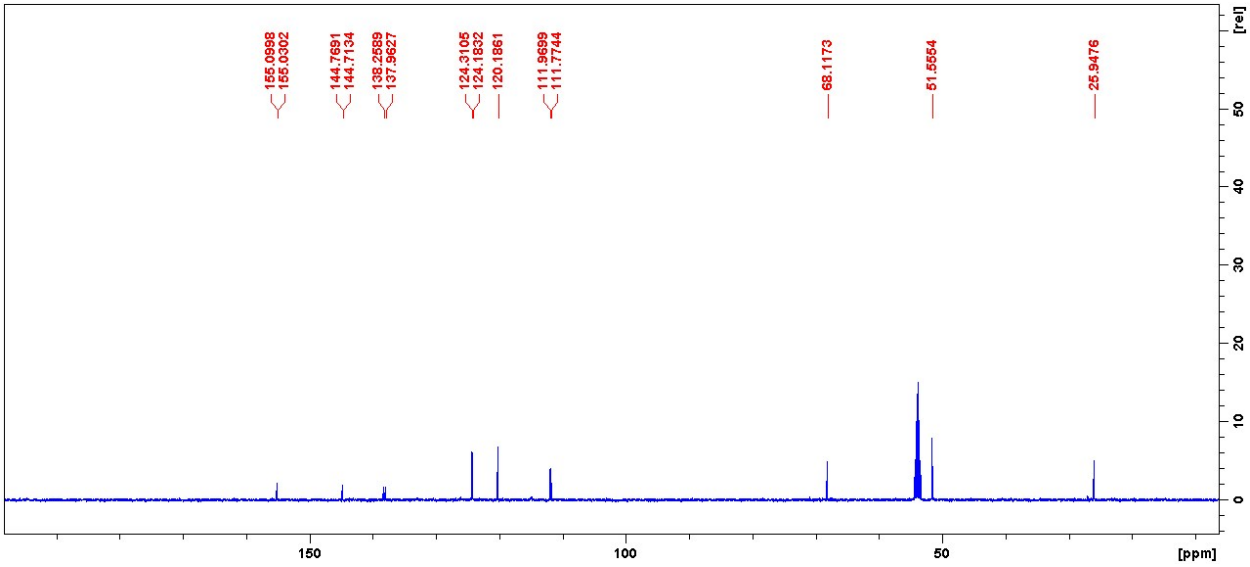
Synthesis of [PF$_2$(BIMEt$_3$)][OTf]$_3$: To a solution of $[P(BIMEt_3)][OTf]_3$ (0.1 mmol, 109 mg) in 3 mL of MeCN, XeF_2 (0.1 mmol, 17 mg) was added to yield a light yellow solution. After stirring for 30 minutes a colourless precipitate was formed, the reaction mixture was filtered and another equivalent of XeF_2 (0.1 mmol, 17 mg) was added, the mixture was layered with 4 mL of diethyl ether and was placed in the freezer for 16 hours to isolate 55 mg of colourless crystals. Total yield: 55 mg (53 %) of the composition $C_{33}H_{33}F_{11}N_7O_9PS_3 \cdot$ MeCN. **MW** = 1048.9 g/mol, **MP** = 251 °C (dec.) **EA [calc.]:** C, 39.33; H, 3.30; N, 9.73. **EA [found.]:** C, 39.38; H, 3.10; N, 9.63. **^{1}H NMR** (300 MHz, MeCN-d3) δ = 8.88 – 8.76 (m, 1H, CH_{arom}), 8.27 – 8.07 (m, CH_{arom}, 2H), 8.27 – 8.07 (m, 2H, CH_{arom}), 8.04 – 7.81 (m, 3H, CH_{arom}), 7.81 – 7.58 (m, 6H, CH_{arom}), 6.45 (dd, *J* = 17.1, 20.2 Hz, 2H, , CH_2), 6.01 (pseudo-t, *J* = 8.0 Hz, 4H, , CH_2), 4.55 (dq, *J* = 1.4, 7.4 Hz, 4H, , CH_2), 4.17 (q, *J* = 7.4 Hz, 2H, CH_2), 1.60 (t, *J* = 7.4 Hz, 6H, CH_3), 1.36 (t, *J* = 7.4 Hz, 3H, CH_3). **^{19}F{^{1}H} NMR** (283 MHz, CD_3CN): δ = -79.3 (s), -65.5 (dd, J_{PF} = 849.7, J_{FF} = 52.0), -33.9 (dd, J_{PF} = 899.3, J_{FF} = 52.0). **^{13}C{^{1}H} NMR** (75.5 MHz CD_3CN): δ = 144.0 (s, *C_{arom}*), 143.5 (s, C_{arom}), 134.7 (d, *J* = 9.2 Hz, C_{arom}), 134.1 (d, *J* = 7.0 Hz, C_{arom}) 128.6 (s, *C_{arom}*), 128.4 (s, C_{arom}), 128.1 (s, *C_{arom}*), 127.9 (s, C_{arom}), 115.0 (d, *J* = 9.2 Hz, C_{arom}), 114.2 (d, *J* = 7.6 Hz, C_{arom}), 114.1 (s, *C_{arom}*), 113.9 (s, *C_{arom}*), 60.5 (s, CH_2), 60.13 (s, CH_2), 42.7 (s, CH_2), 42.38 (s, CH_2), 12.97 (s, CH_3), 11.93 (s, CH_3). **^{31}P{^{1}H} NMR** (121.4 MHz , CD_3CN): δ = -127.8 (dd, J_{PF} = 899.3, 849.7 Hz)

Traces of moisture leads to decomposition of the product and the formation of $[HBIMEt_3][PF_6]$ indicated by the formation of a *septed*-resonance in the ^{31}P-NMR spectrum for the PF_6-anion (-144.6 ppm, $^1J_{P,F}$ = 706.3 Hz). Scaling up the reaction only yielded several side products. Decomposition of the product in solution was observed if left in MeCN overnight, crystallization has to be initiated right after addition of XeF_2 to isolate crystalline material of the $[PF_2(BIMEt_3)][OTf]_3$.

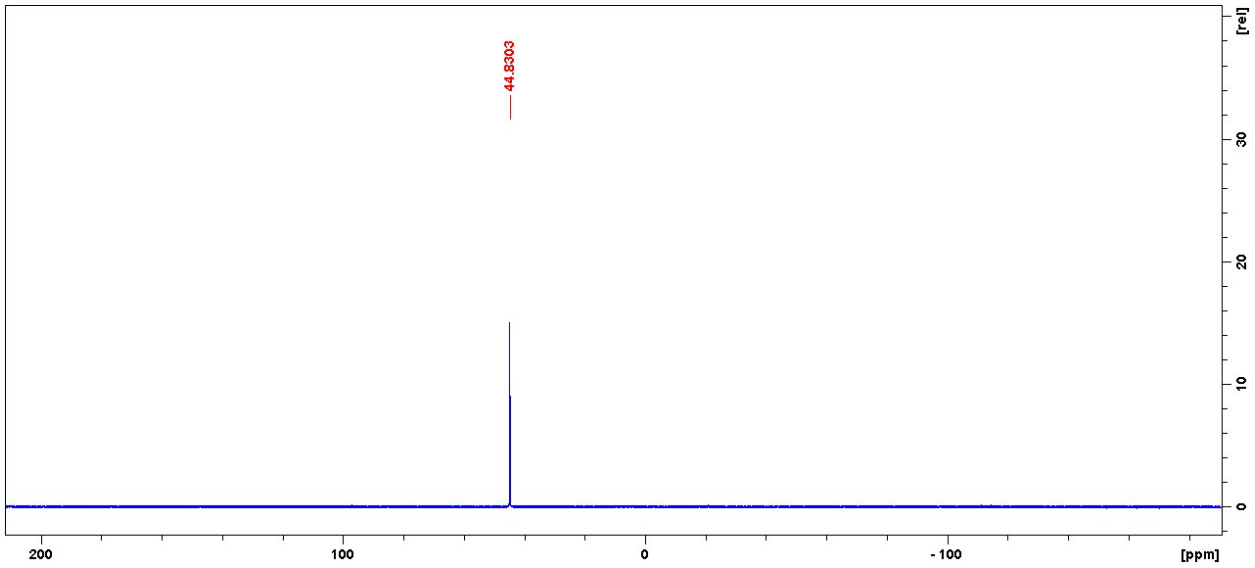
NMR spectra



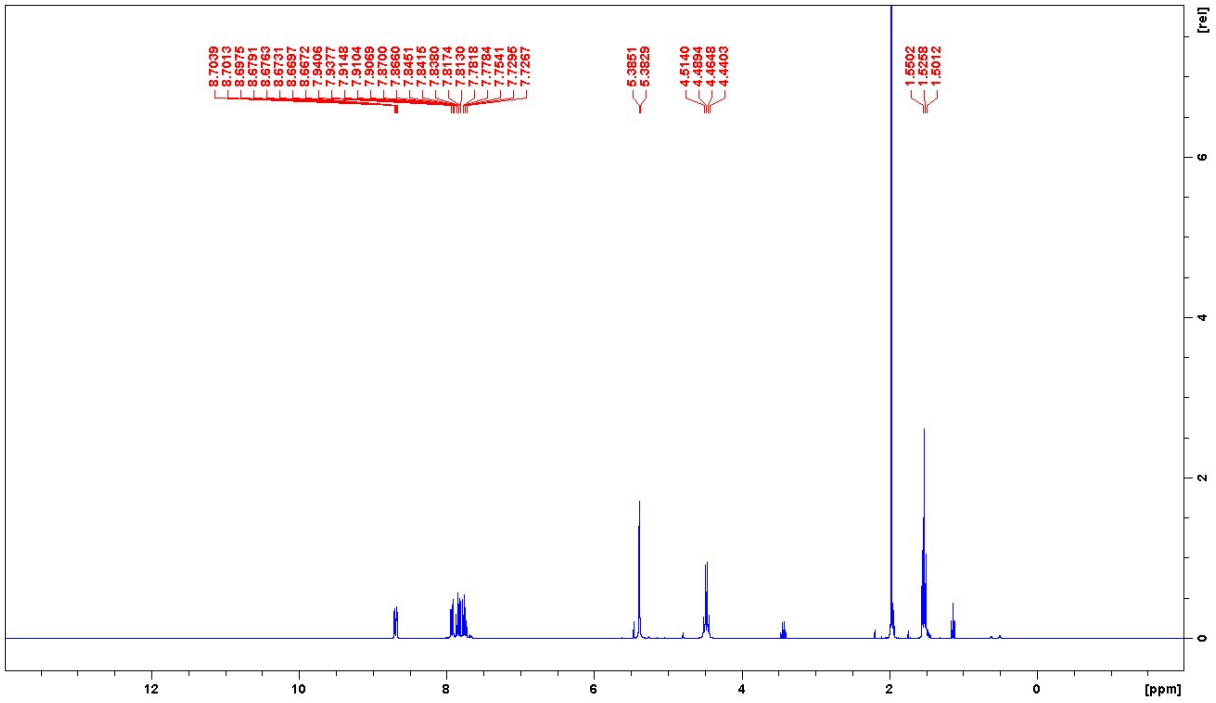
Scheme S1: ^{1}H NMR of PBIM



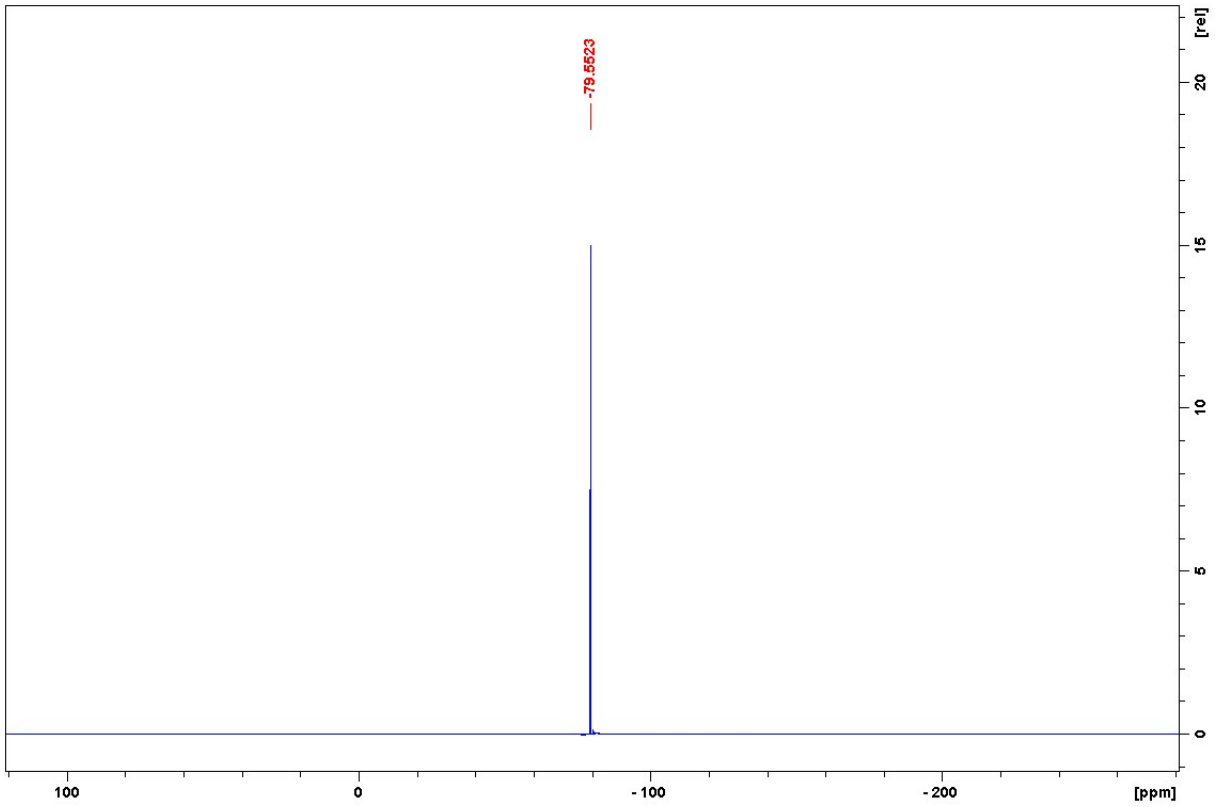
Scheme S2: ^{13}C NMR of PBIM



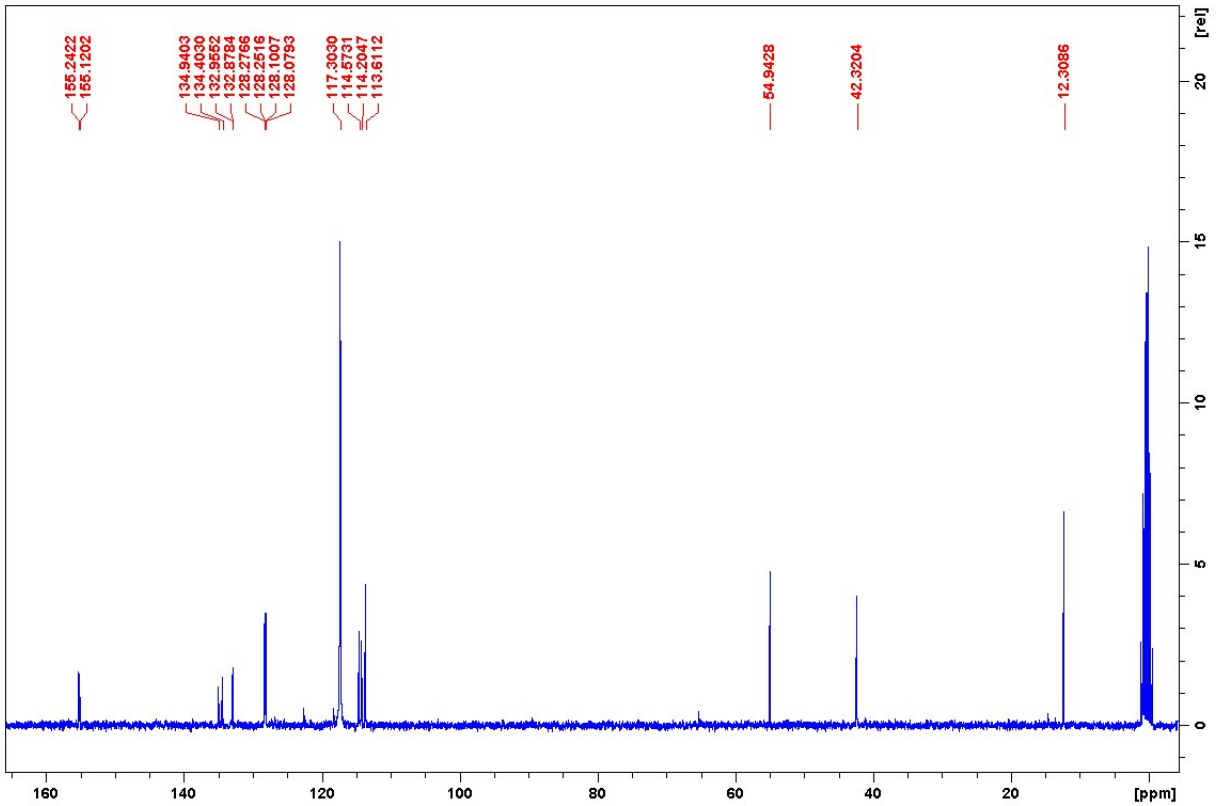
Scheme S3: ^{31}P NMR of PBIM



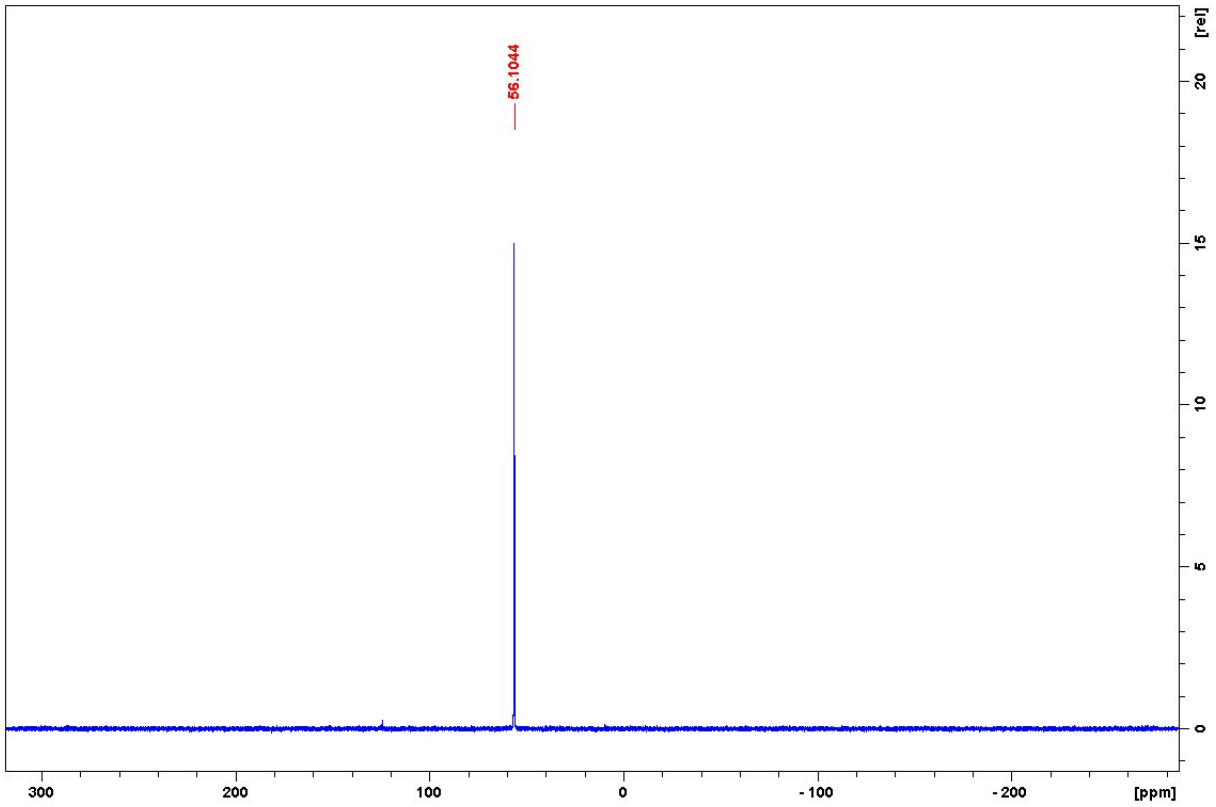
Scheme S4: ^{1}H NMR of $[P(BIMEt_3)][OTf]_3$



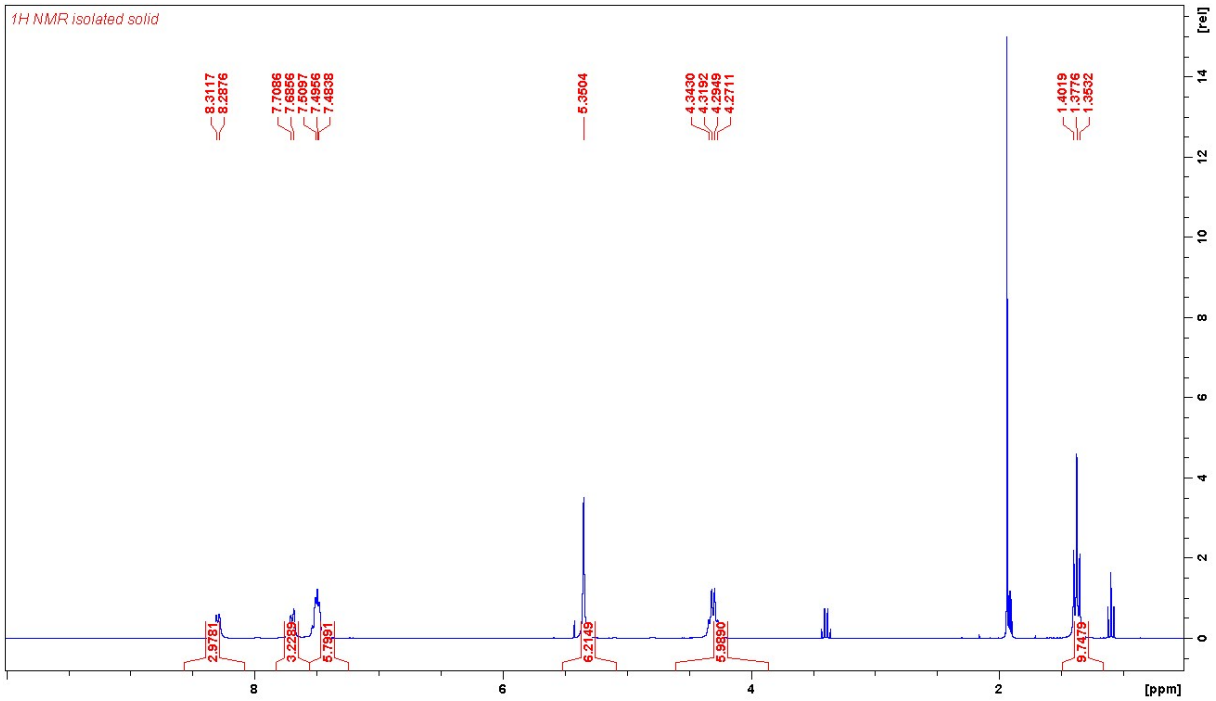
Scheme S5: ^{19}F NMR of $[P(BIMEt_3)][OTf]_3$



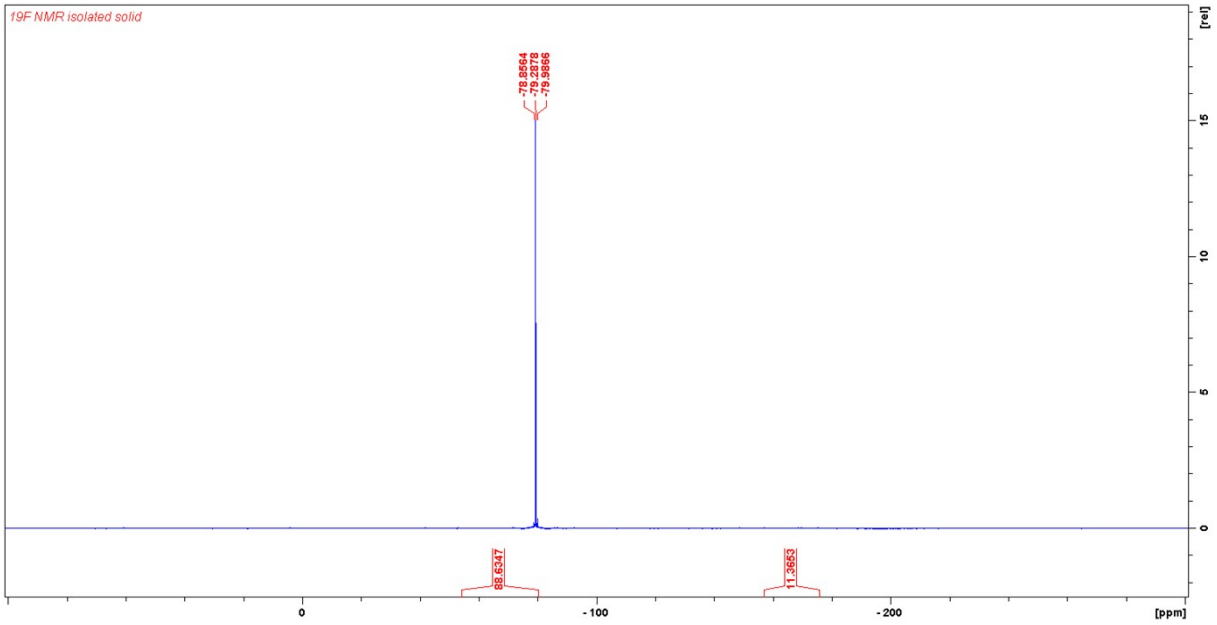
Scheme S6: ^{13}C NMR of $[P(BIMEt_3)][OTf]_3$



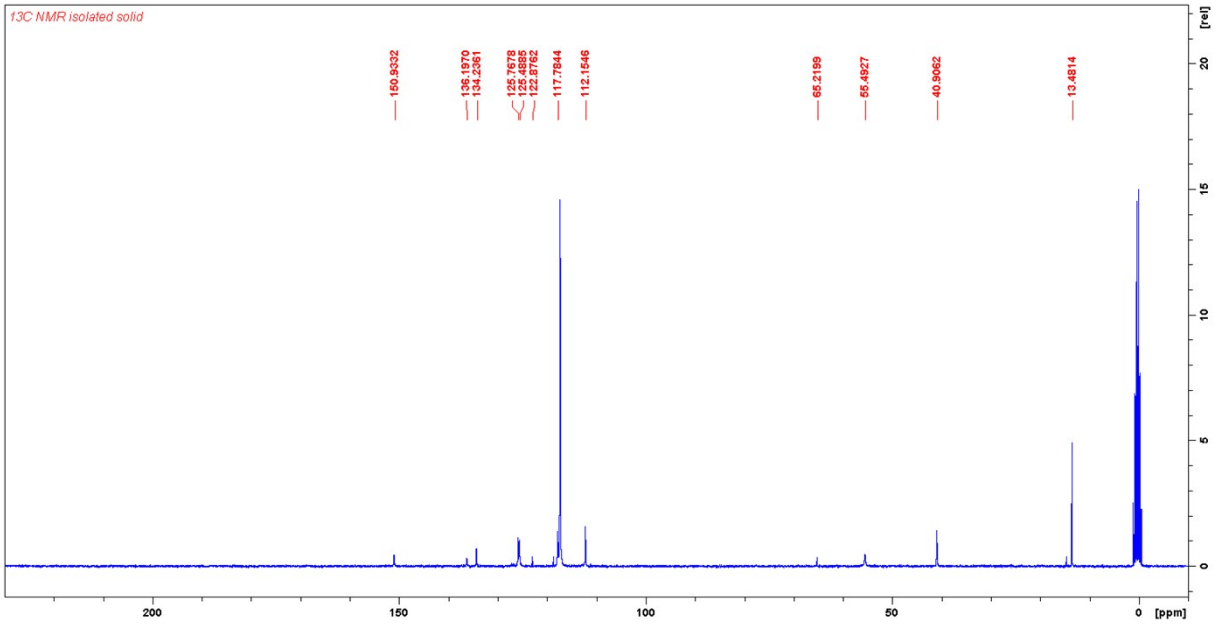
Scheme S7: ^{31}P NMR of $[P(BIMEt_3)][OTf]_3$



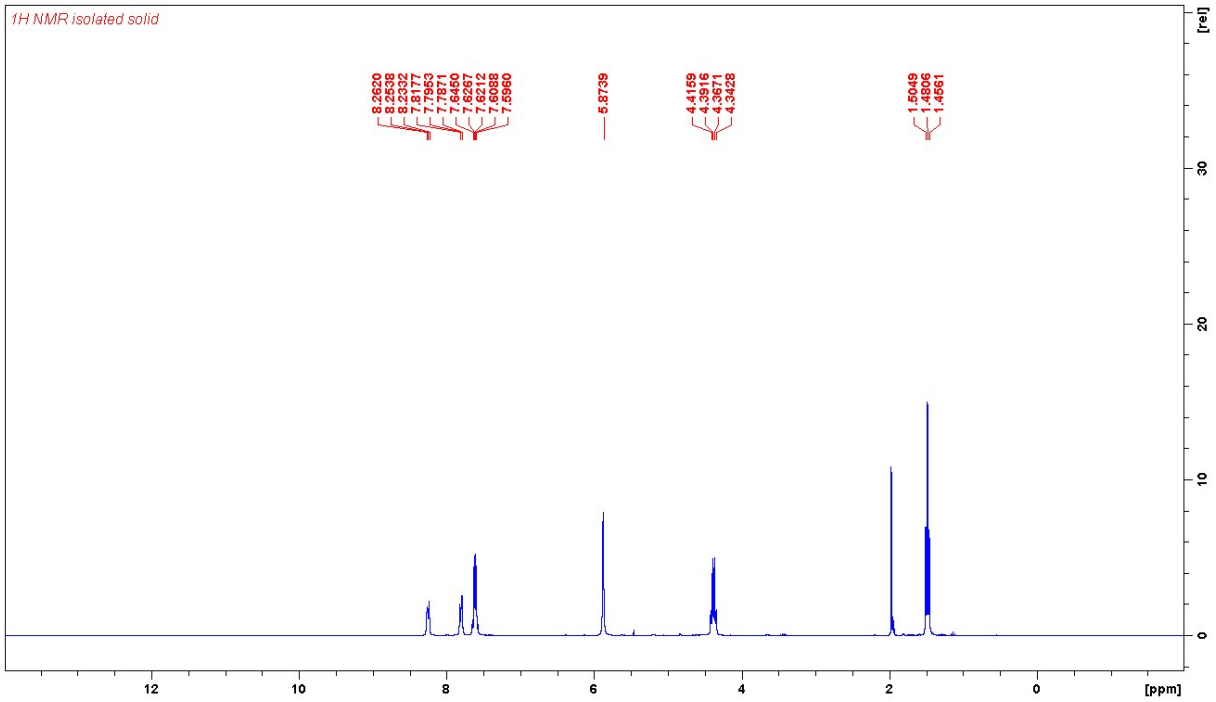
Scheme S8: ^{1}H NMR of $[AsCl(BIMEt_3)][OTf]_2$



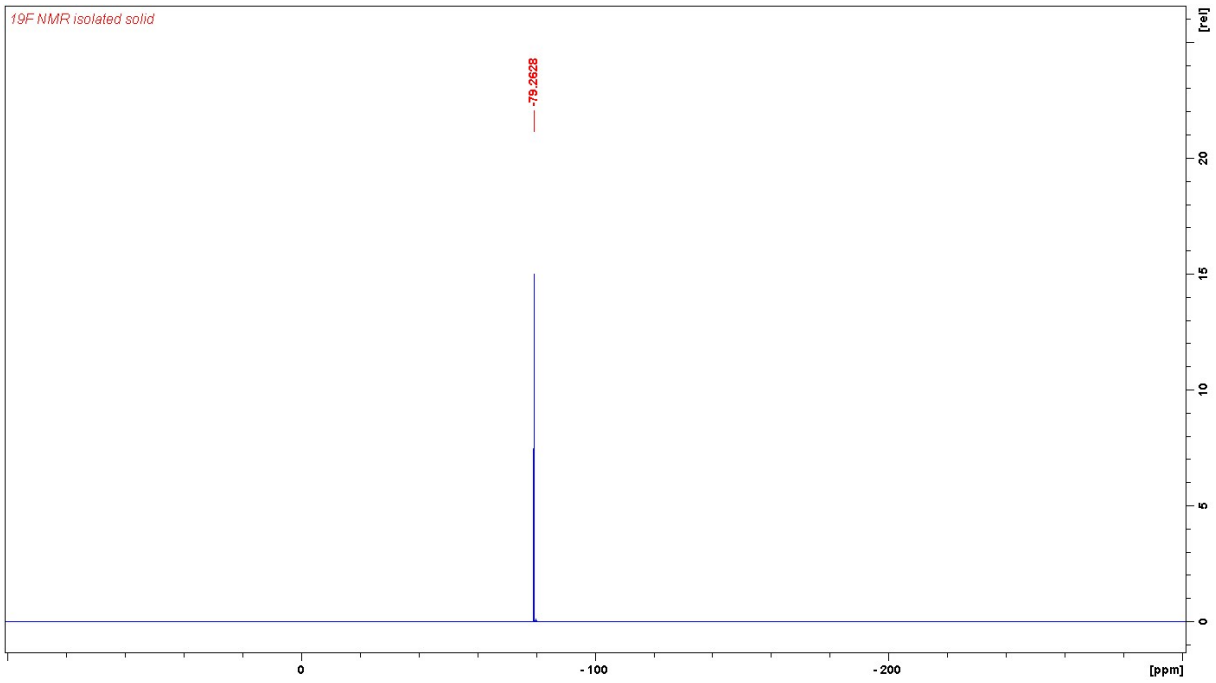
Scheme S9: ^{19}F NMR of $[AsCl(BIMEt_3)][OTf]_2$



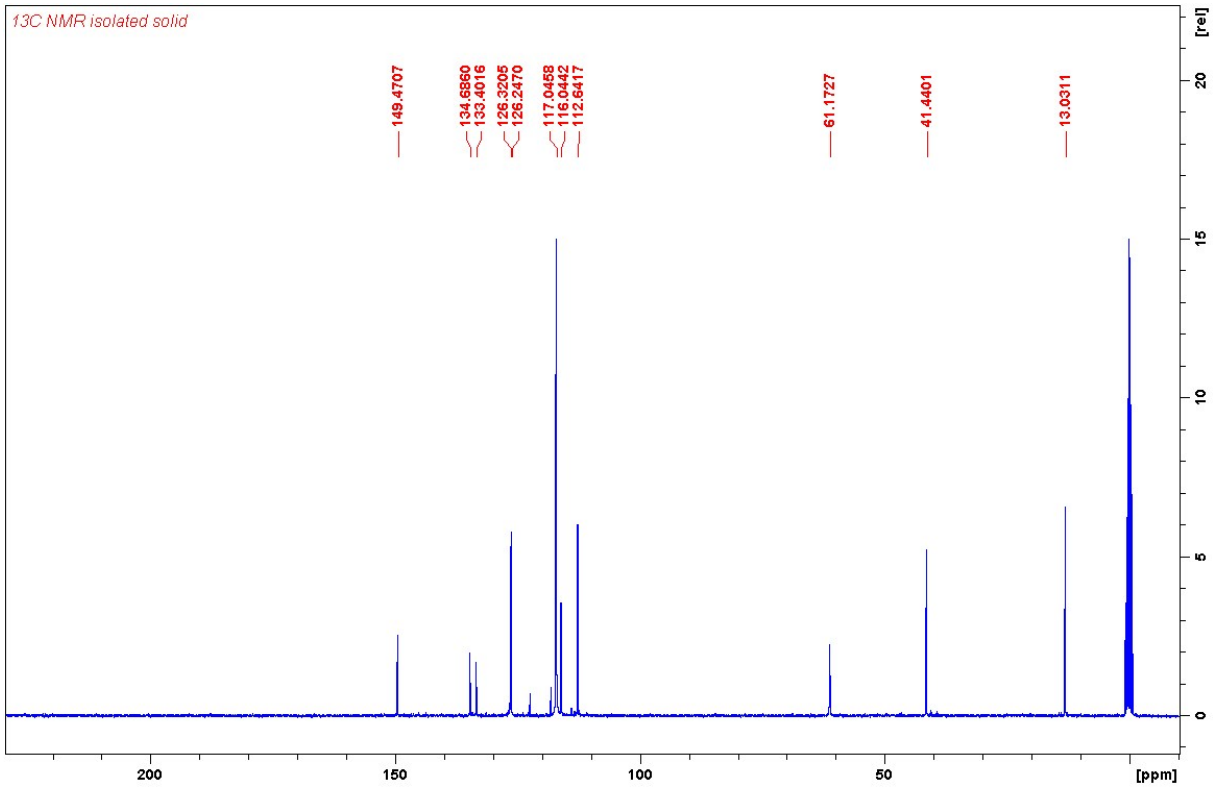
Scheme S10: ^{13}C NMR of $[AsCl(BIMEt_3)][OTf]_2$



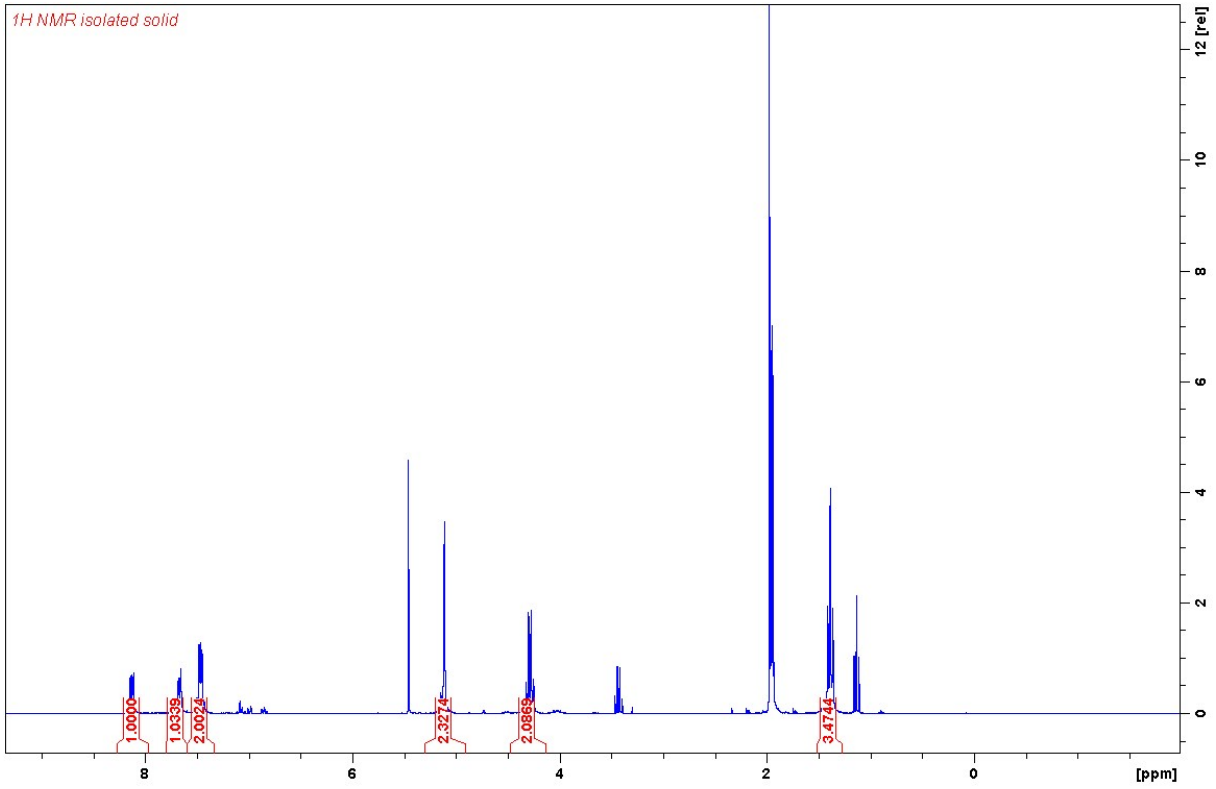
Scheme S11: ^{1}H NMR of [As(BIMEt$_3$)][OTf]$_3$



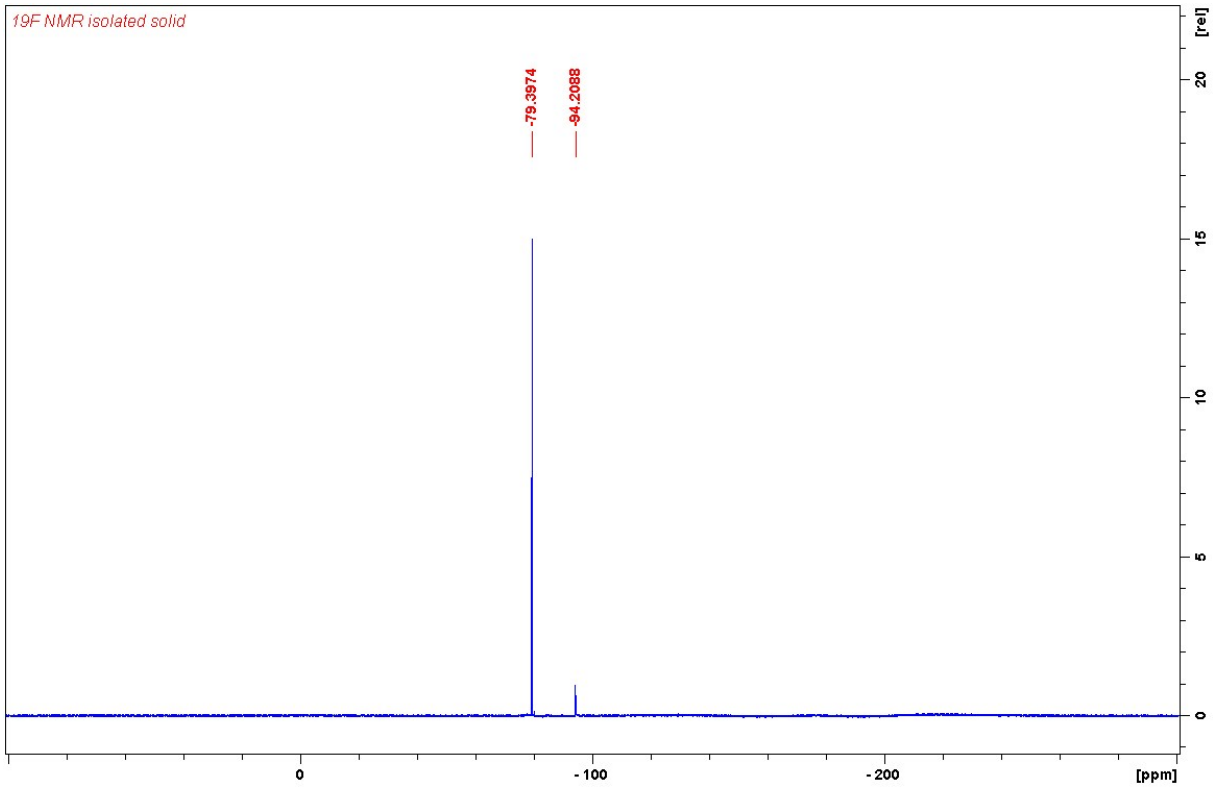
Scheme S12: ^{19}F NMR of [As(BIMEt$_3$)][OTf]$_3$



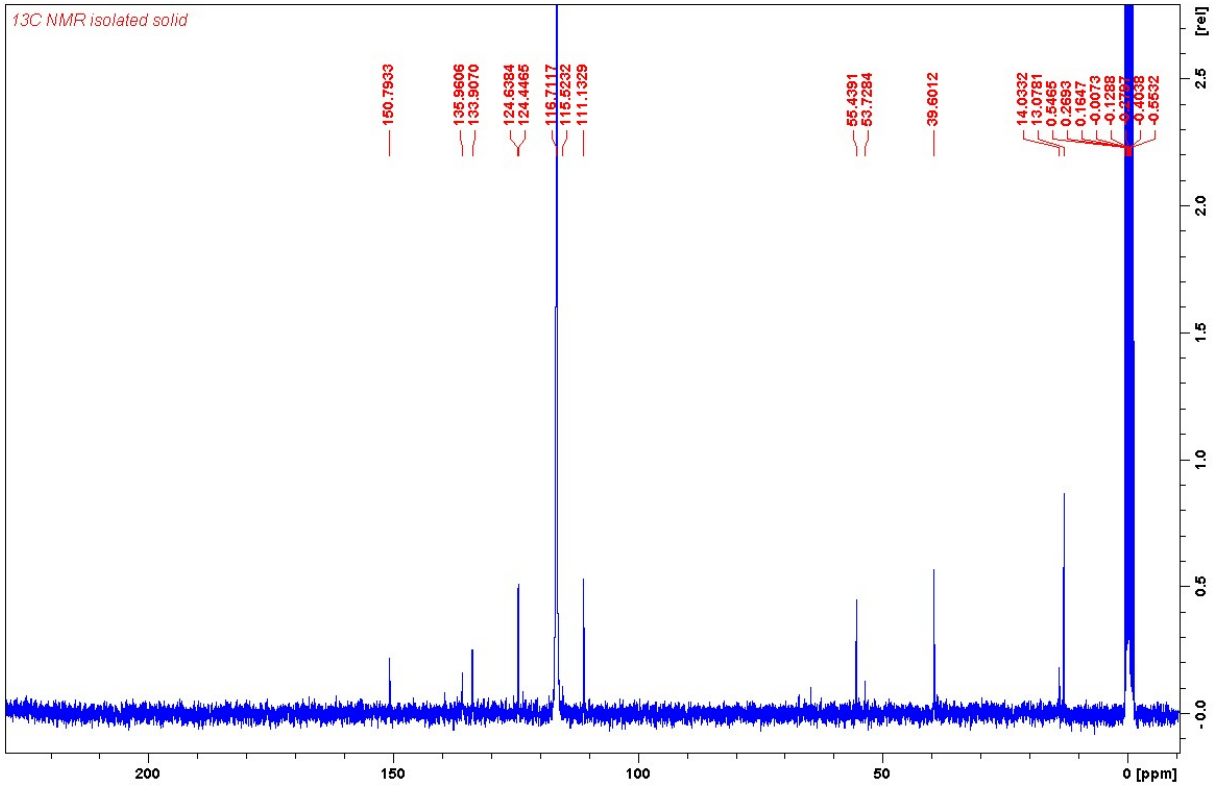
Scheme S13: ^{13}C NMR of $[As(BIMEt_3)][OTf]_3$



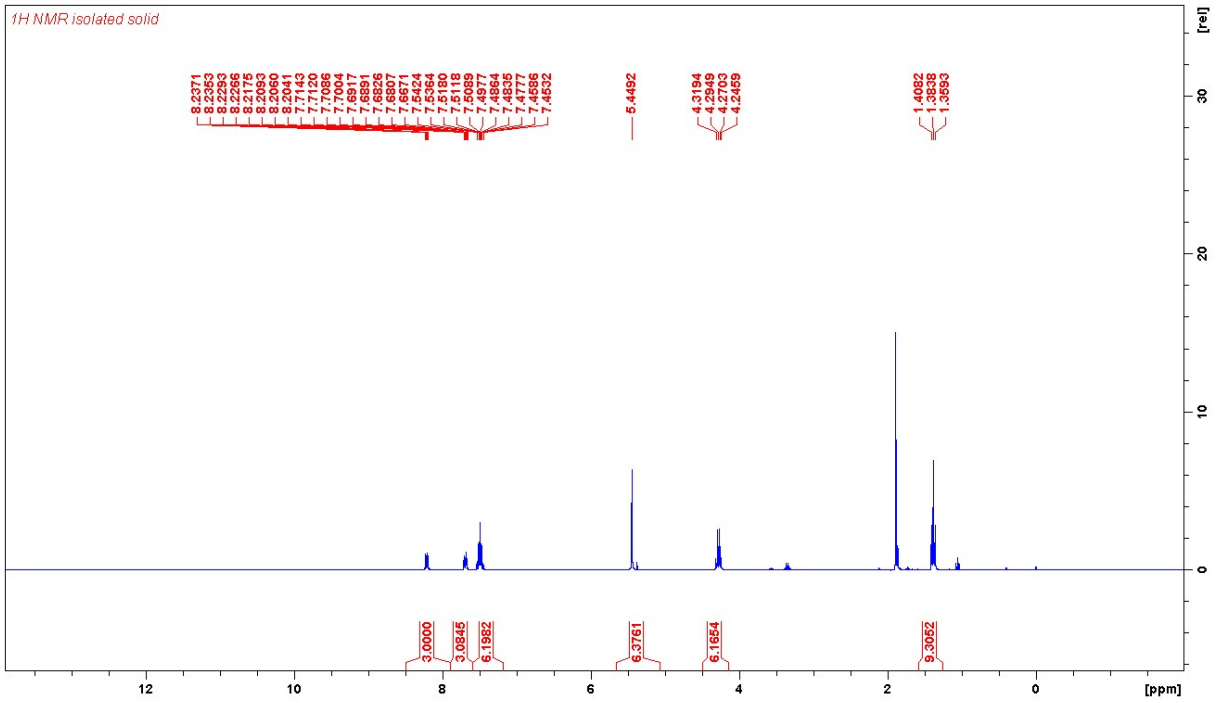
Scheme S14: ^{1}H NMR of $[SbF(BIMEt_3)][OTf]_2$



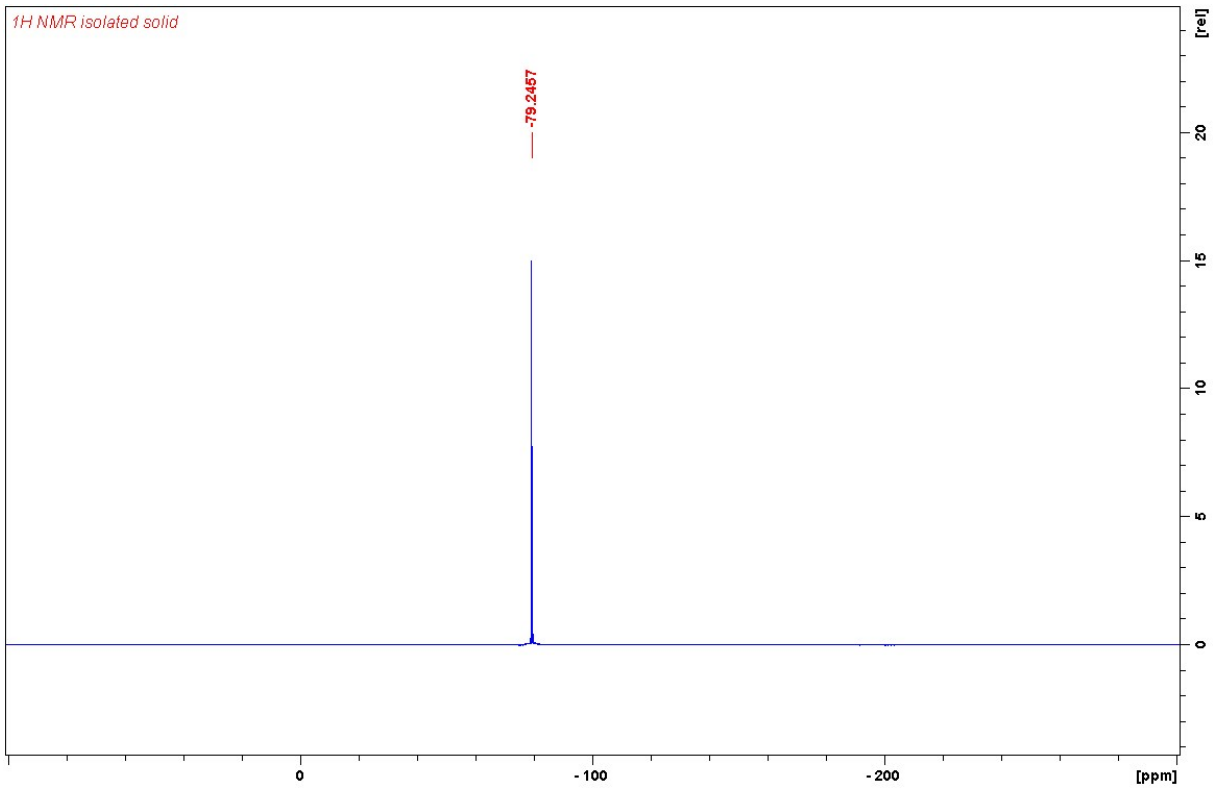
Scheme S15: ^{19}F NMR of $[SbF(BIMEt_3)][OTf]_2$



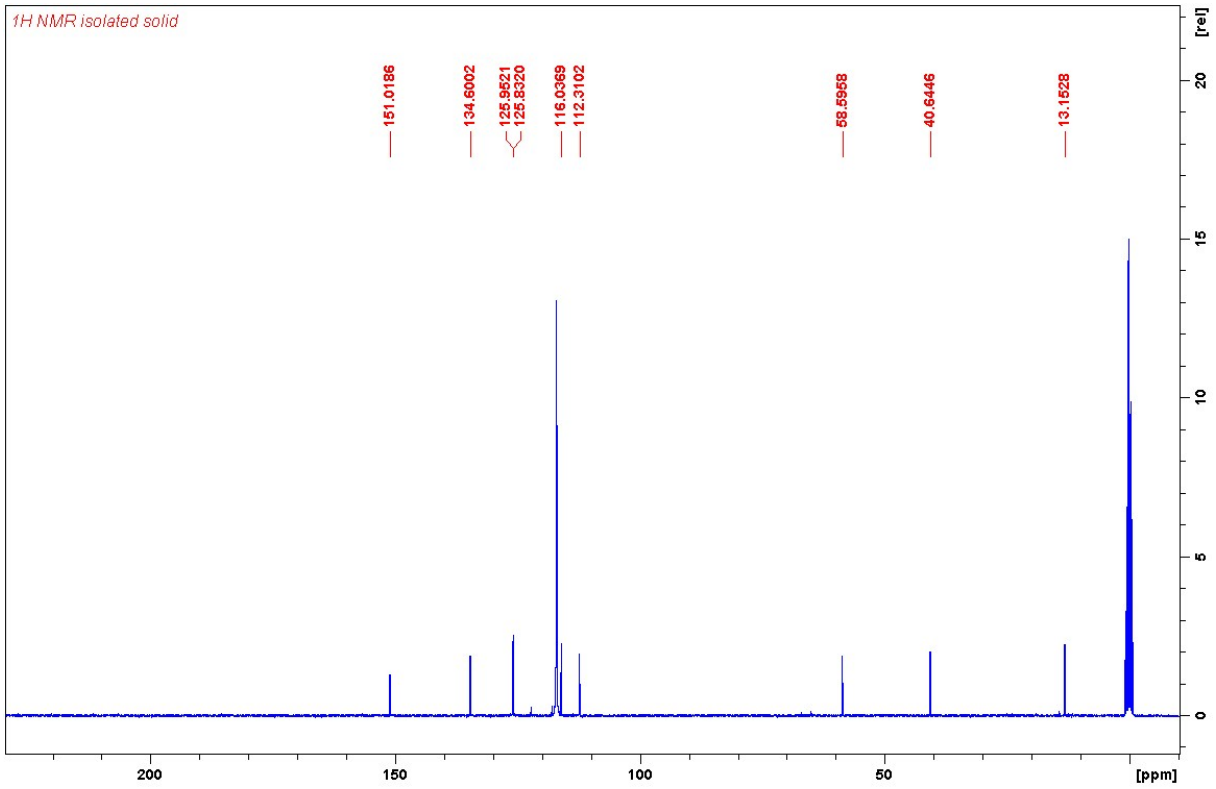
Scheme S16: ^{13}C NMR of $[SbF(BIMEt_3)][OTf]_2$



Scheme S17: ^{1}H NMR of [Sb(BIMEt$_3$)][OTf]$_3$

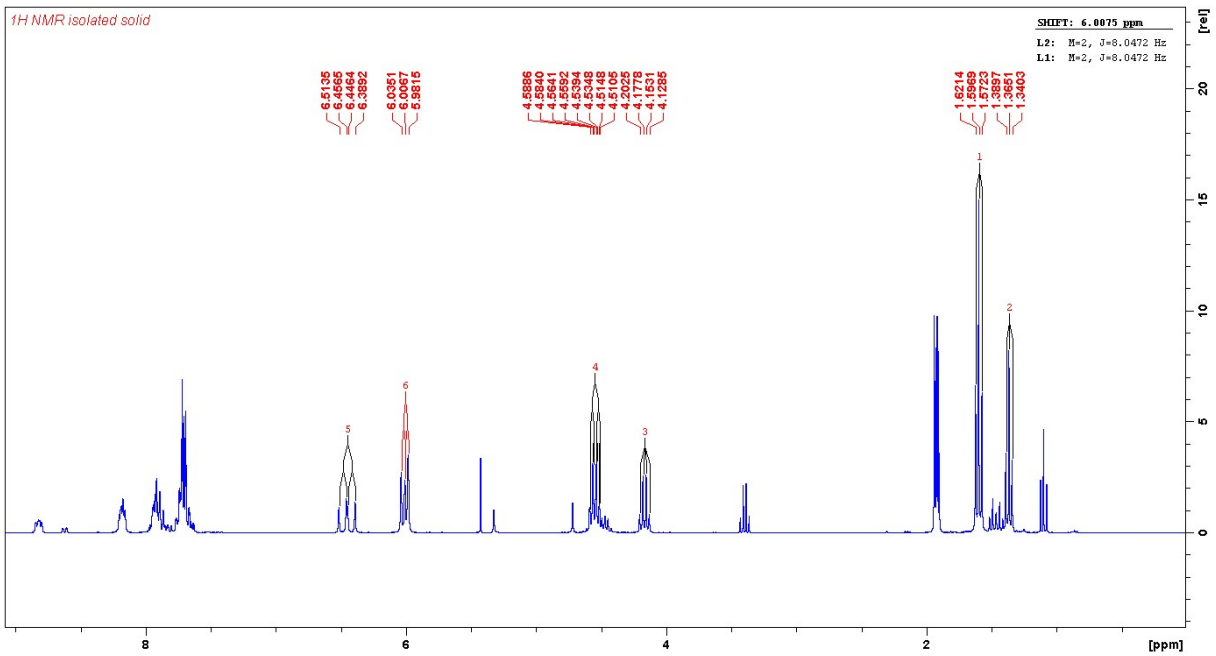


Scheme S18: ^{19}F NMR of [Sb(BIMEt$_3$)][OTf]$_3$

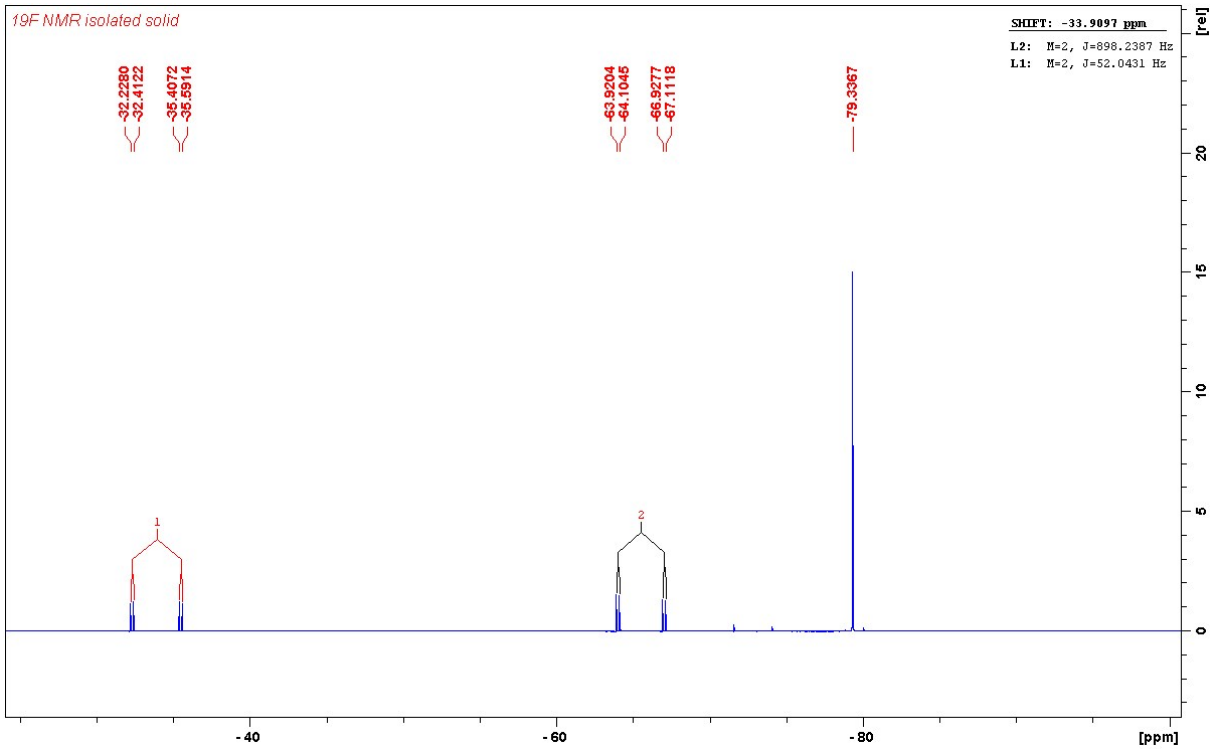


Scheme S19: ^{13}C NMR of $[Sb(BIMEt_3)][OTf]_3$

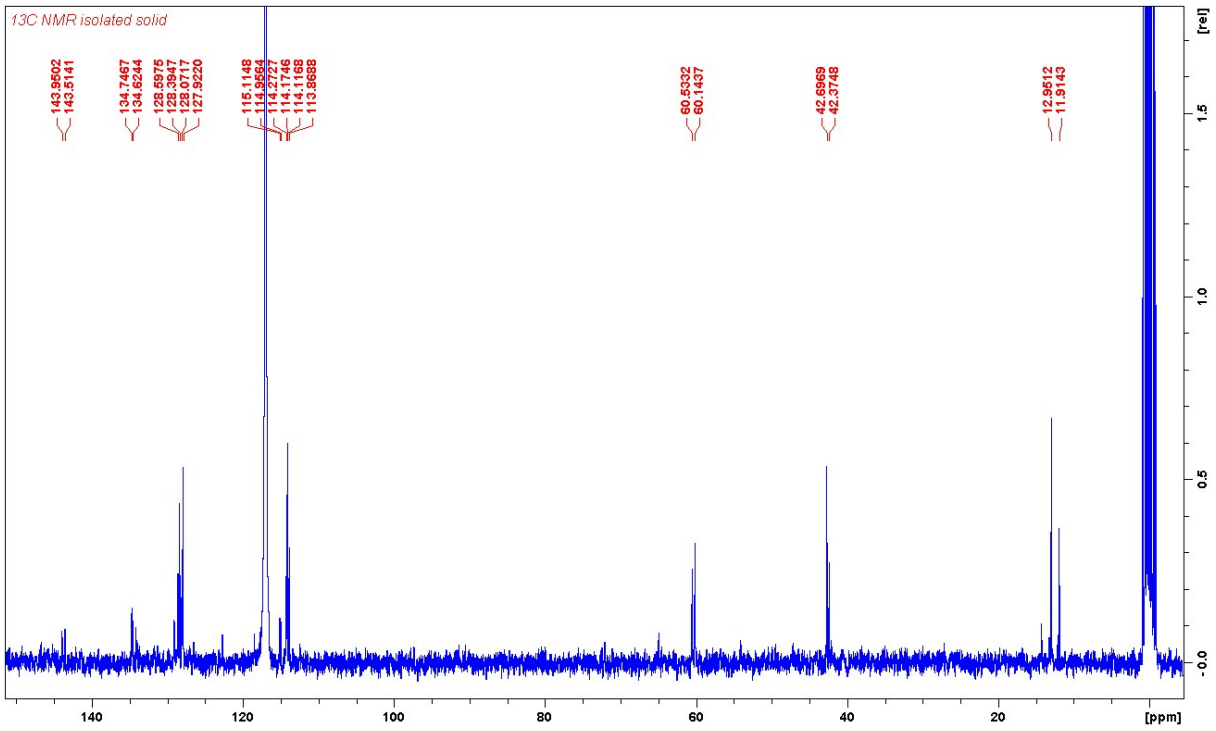
$[PF_2BIMEt_3][OTf]_3$



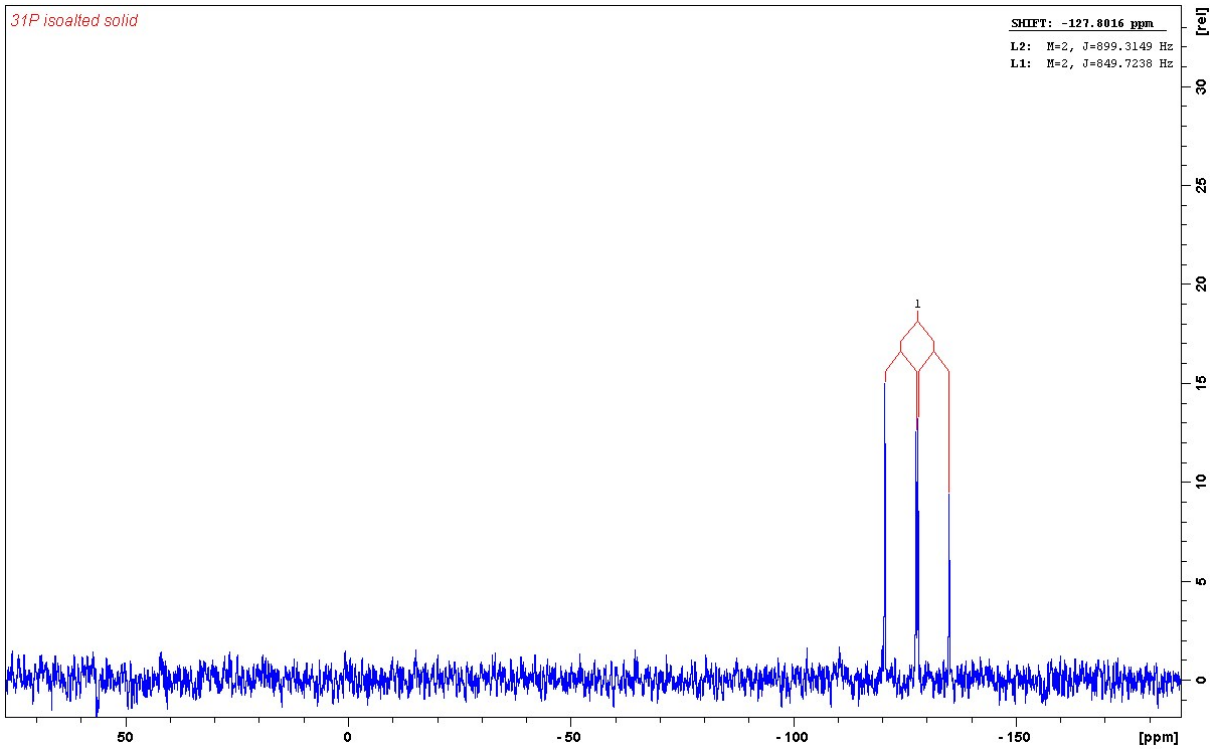
Scheme S20: ^{1}H NMR of $[PF_2(BIMEt_3)][OTf]_3$



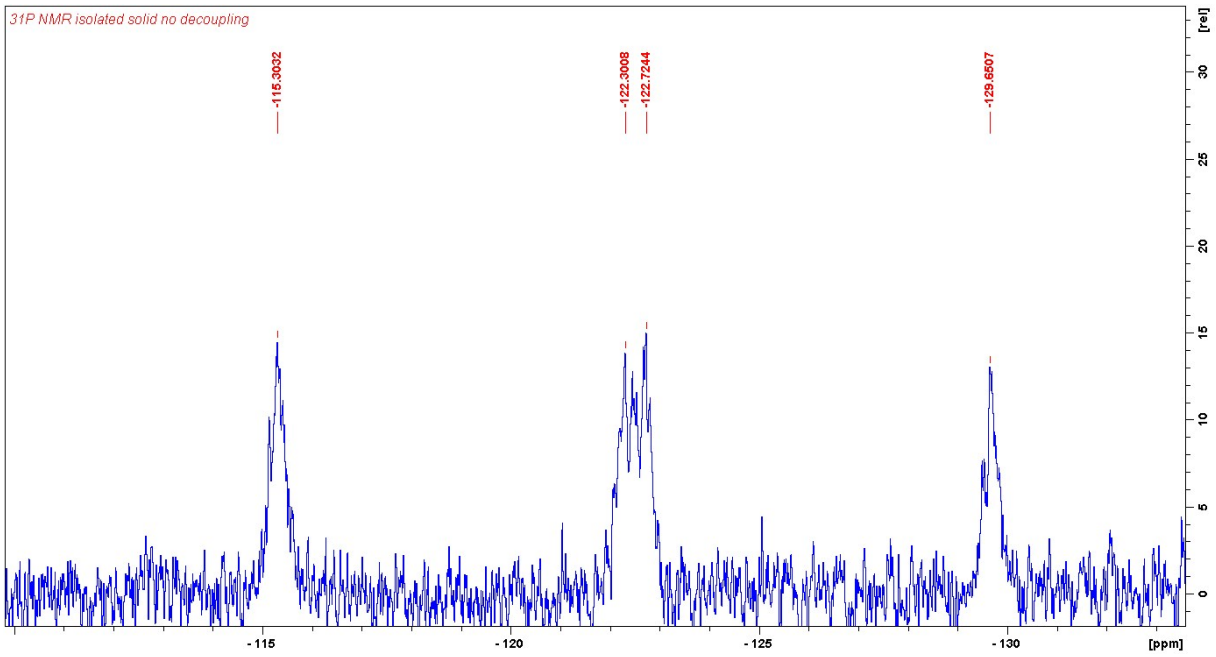
Scheme S21: ^{19}F NMR of $[PF_2(BIMEt_3)][OTf]_3$



Scheme S22: ^{13}C NMR of $[PF_2(BIMEt_3)][OTf]_3$



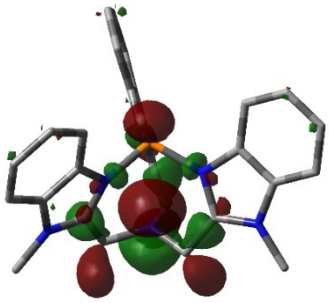
Scheme S23: $^{31}P\{^{1}H\}$ NMR of $[PF_2(BIMEt_3)][OTf]_3$



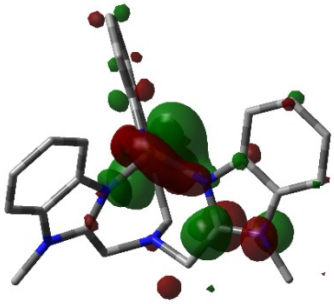
Scheme S24: ^{31}P NMR of $[PF_2(BIMEt_3)][OTf]_3$

Calculations Details

Structure optimization of $[P(BIMMe_3)]^{3+}$ implies a significant electron donation from the tertiary amine into the P^{3+} cation based on its geometry. The lone pair at nitrogen is best described as the HOMO-6 but shows only a weak interaction with the phosphorus centre. The HOMO of the tricationic phosphorus complex is exclusively located on the aromatic backbone of the benzoimidazole substituents and not on the phosphorus lone pair. The LUMO on the other hand is best described as a δ^*-orbital for one of the nitrogen phosphorus bonds of the benzoimidazole unit, indicating the cleavage of the bond upon reaction with a nucleophile.



HOMO -6



LUMO

Figure S1: Optimized gas phase structures on the PBEPBE/6-311+G(d,p) level of theory for $[P(BIMMe_3)]^{3+}$.

Table S1: Summarized energies for optimized structures in the acetonitrile solvent field of methylated species of [BIMP] on the PBEPBE/6-311+G(d,p) level of theory and the corresponding energy diagram. N-Methylation represents the methylation solely at the nitrogen atoms, P-Methylation shows the energy for compounds methylated at least ones at phosphorus.

N-Methylation	eV	P-Methylation	eV
[BIMP]	0	[BIMP]	0
+ 4 Me^+		+ 4 Me^+	
$[BIMMeP]^+$	-3.83	$[BIMPMe]^+$	-3.41
+ 3 Me^+		+ 3 Me^+	
$[BIMMe_2P]^{2+}$	-7.48	$[BIMMePMe]^{2+}$	-6.82
+ 2 Me^+		+ 2 Me^+	
$[BIMMe_3P]^{3+}$	-10.91	$[BIMMe_2PMe]^{3+}$	-10.07
+ 1 Me^+		+ 1 Me^+	
$[BIMMe_3PMe]^{4+}$	No min,	$[BIMMe_3PMe]^{4+}$	No min

NBO analysis of $[BIMMe_3P]^{3+}$

Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population			
			Core	Valence	Rydberg	Total
P	1	1.40945	9.99854	3.54612	0.04589	13.59055
N	2	-0.55305	1.99943	5.53395	0.01967	7.55305
N	3	-0.30677	1.99910	5.29431	0.01336	7.30677
N	4	-0.65195	1.99919	5.63054	0.02223	7.65195
N	5	-0.30740	1.99910	5.29491	0.01339	7.30740
N	6	-0.65053	1.99919	5.62898	0.02237	7.65053
N	7	-0.30600	1.99910	5.29379	0.01310	7.30600
N	8	-0.65152	1.99919	5.63078	0.02155	7.65152

Wiberg bond index matrix in the NAO basis:

Atom		1	2	3	4	5	6	7	8	9
1.	P	0.0000	0.0359	0.0219	0.7354	0.0220	0.7356	0.0219	0.7353	0.0016
2.	N	0.0359	0.0000	0.0069	0.0114	0.0069	0.0113	0.0069	0.0114	0.9652
3.	N	0.0219	0.0069	0.0000	0.0856	0.0004	0.0041	0.0004	0.0014	0.0114
4.	**N**	**0.7354**	0.0114	0.0856	0.0000	0.0015	0.0214	0.0041	0.0216	0.0095
5.	N	0.0220	0.0069	0.0004	0.0015	0.0000	0.0856	0.0004	0.0041	0.0005
6.	**N**	**0.7356**	0.0113	0.0041	0.0214	0.0856	0.0000	0.0015	0.0215	0.0007
7.	N	0.0219	0.0069	0.0004	0.0041	0.0004	0.0015	0.0000	0.0856	0.0007
8.	**N**	**0.7353**	0.0114	0.0014	0.0216	0.0041	0.0215	0.0856	0.0000	0.0010

Coordinates of optimized structures in gas phase

$[BIMMe2P]^{2+}$

P	0.00139042	0.27232047	0.58182607
N	0.06504819	-0.15333556	-2.32899576
N	-0.81704714	3.30469363	-1.83720319
N	-0.43038893	1.67981243	-0.29095337
N	-2.67578218	-2.22824584	-1.02904578
N	-1.08778190	-1.08274524	0.00817000
N	3.36770036	-1.12863987	-1.08988634
N	1.62951262	-0.24349333	-0.04191630
C	0.30901587	1.24447182	-2.67263126
H	-0.05055651	1.53086535	-3.67610758
H	1.39985055	1.41105784	-2.66979145
C	-1.27700135	-0.66240757	-2.47033206
H	-1.39576831	-1.36803236	-3.31465448
H	-1.95288415	0.18474014	-2.68083754
C	1.17138340	-1.07556609	-2.38038511
H	1.76219062	-0.99561597	-3.31251883
H	0.79304657	-2.11207974	-2.34560595
C	-0.34003609	2.11649727	-1.65045075
C	-1.25736606	3.75959413	-0.59148093
C	-1.85152707	4.98224305	-0.26361484
H	-2.01624906	5.73893579	-1.03117376
C	-2.21298328	5.18684803	1.06658906
H	-2.67571397	6.12987548	1.35967796
C	-1.99228180	4.19960805	2.04456708
H	-2.28836030	4.39555141	3.07598327
C	-1.40320730	2.96981384	1.73294237
H	-1.24632166	2.21842821	2.50840953
C	-1.03758299	2.77922615	0.40203402
C	-1.69685408	-1.32274662	-1.18868250
C	-2.73619922	-2.60701668	0.32034450
C	-3.57129303	-3.50827994	0.98298980
H	-4.35085784	-4.06874781	0.46659345
C	-3.35864897	-3.65572238	2.35186284
H	-3.98568342	-4.34644808	2.91657663
C	-2.35396220	-2.93206478	3.02478817
H	-2.22392652	-3.07913949	4.09757371
C	-1.52052986	-2.03345755	2.35976736
H	-0.74869794	-1.48133066	2.89527194
C	-1.73280967	-1.88060343	0.98763072
C	2.06085409	-0.83389582	-1.19338572
C	3.83250198	-0.72576936	0.17020230
C	5.10154053	-0.80335853	0.74710953
H	5.95344032	-1.23999513	0.22549589
C	5.22752913	-0.28584740	2.03413838
H	6.19870292	-0.32009285	2.52893618
C	4.13070328	0.28414215	2.71133902
H	4.27733682	0.68232413	3.71599967
C	2.86433628	0.35987014	2.13312345
H	2.02954680	0.81266681	2.66765792
C	2.73313292	-0.16366394	0.84447423
C	-3.58608644	-2.74005962	-2.05918860
H	-3.53088633	-3.83595419	-2.08111097
H	-4.61231352	-2.42700588	-1.82521960
H	-3.30956775	-2.34356610	-3.04056372
C	4.21464473	-1.78066457	-2.09457720
H	5.07449822	-1.13552441	-2.31637111
H	4.56758241	-2.74420844	-1.70388103
H	3.64827185	-1.95497670	-3.01395905

$[BIMMe_2PMe]^{3+}$

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N	-0.38681111	1.77995406	-0.27236818
N	-1.22889098	-1.10439444	0.00336844
N	3.24353570	-1.51026719	-1.16521339
N	1.68548723	-0.38096857	-0.05238039
C	0.49547999	1.23503545	-2.52096413
H	0.19491499	1.39360367	-3.56814660
H	1.59739638	1.24557192	-2.47497684
C	-1.39368961	-0.36122353	-2.33616351

H	-1.47866465	-0.90140470	-3.29291105
H	-1.92616657	0.59993128	-2.44126785
C	0.94652769	-1.20290672	-2.25123789
H	1.36679493	-1.14972648	-3.26817635
H	0.40246899	-2.15775776	-2.15714461
C	-0.10365480	2.24174735	-1.60993148
C	-0.83810100	3.97408680	-0.58002156
C	-1.27403807	5.27091868	-0.30124066
H	-1.22481904	6.04220520	-1.07105433
C	-1.77014988	5.52618362	0.97615956
H	-2.11717887	6.52810141	1.23169910
C	-1.84328865	4.50643287	1.93870812
H	-2.25449725	4.73101173	2.92399369
C	-1.41652592	3.19753236	1.67480884
H	-1.52362427	2.44432669	2.45197885
C	-0.88682677	2.95440384	0.40900169
C	-1.91447754	-1.14587528	-1.18409041
C	-3.04393990	-2.44861506	0.21545151
C	-3.96267272	-3.33596403	0.77659611
H	-4.82089671	-3.71328530	0.21917786
C	-3.72381230	-3.72912650	2.09071115
H	-4.41351548	-4.42017895	2.57728788
C	-2.59746648	-3.26519181	2.79617827
H	-2.42892490	-3.61590326	3.81552646
C	-1.67669044	-2.38004782	2.23139600
H	-0.80898961	-2.07340872	2.80915711
C	-1.92771575	-1.94799359	0.92656641
C	1.98960855	-1.07077794	-1.19682395
C	3.83376009	-1.09483634	0.04159048
C	5.13627790	-1.28506914	0.50447672
H	5.87536657	-1.85603646	-0.05881971
C	5.45461991	-0.69425341	1.72398472
H	6.46032005	-0.81100747	2.13008770
C	4.50708306	0.06841124	2.43281738
H	4.80102860	0.53936403	3.37212858
C	3.20399574	0.25888864	1.96842556
H	2.52143831	0.88111619	2.54031796
C	2.86355107	-0.35813931	0.76207132
C	3.94038910	-2.29578246	-2.19701293
H	4.82204727	-1.73846059	-2.53949660
H	4.25167444	-3.25690396	-1.76709060
H	3.27319957	-2.48213629	-3.04469932
P	0.00665718	0.20643609	0.20974800
C	0.00022655	0.33206065	2.01801003
H	0.46015660	1.28734730	2.30191492
H	-1.03557941	0.32172399	2.38064944
H	0.55598906	-0.49613710	2.47237216
N	-2.98745869	-1.92291975	-1.08827331
C	-3.98087890	-2.20230127	-2.13844210
H	-3.70532635	-1.68768066	-3.06471070
H	-4.02374088	-3.28447942	-2.31717311
H	-4.96320548	-1.84070358	-1.80664616

$[BIMMe_3PMe]^{3+}$

P	0.00001056	0.00006296	0.63773187
N	0.00045915	0.00059849	-2.25530284
N	-1.69605780	-3.08866248	-1.20817033
N	-0.64301599	-1.52378114	-0.04524152
N	3.52357155	0.07603690	-1.20723808
N	1.64150549	0.20511258	-0.04467895
N	-1.82664906	3.01397751	-1.20714947
N	-0.99821419	1.31890385	-0.04497897
C	-1.05028173	-0.97774526	-2.47508908
H	-0.89509587	-1.57756383	-3.39039891
H	-2.01097521	-0.45285006	-2.61474534
C	1.37310130	-0.42028095	-2.47470211
H	1.81529021	0.01402715	-3.38985036
H	1.39888768	-1.51471557	-2.61437165
C	-0.32141538	1.39979592	-2.47470652
H	-0.91870017	1.56548666	-3.38981956
H	0.61342267	1.96947127	-2.61438911
C	-1.14138686	-1.87344391	-1.27518957
C	-1.57948117	-3.58458607	0.10142783

C	-1.99456622	-4.79574925	0.65854065
H	-2.51265019	-5.55983305	0.07820529
C	-1.71003716	-4.98230808	2.00926994
H	-2.01336057	-5.91105709	2.49426546
C	-1.03815316	-3.99989007	2.76500406
H	-0.83410389	-4.19159289	3.81934209
C	-0.62243012	-2.79096817	2.20540041
H	-0.09876381	-2.04928443	2.80854422
C	-0.91328548	-2.59916061	0.85388910
C	2.19385809	-0.05145899	-1.27452285
C	3.89440024	0.42468152	0.10251683
C	5.15070699	0.67076012	0.65989815
H	6.07158539	0.60426434	0.07974270
C	5.16973966	1.01017729	2.01069611
H	6.12561296	1.21189074	2.49589561
C	3.98287215	1.10044155	2.76625828
H	4.04664003	1.37276716	3.82067113
C	2.72818357	0.85593042	2.20640032
H	1.82395273	0.93826426	2.80946350
C	2.70773975	0.50856725	0.85476446
C	-1.05149545	1.92608711	-1.27457206
C	-2.31493030	3.16007748	0.10237131
C	-3.15679340	4.12452355	0.65978861
H	-3.55948406	4.95549956	0.07984288
C	-3.46123327	3.97034224	2.01026292
H	-4.11434570	4.69686223	2.49545763
C	-2.94648938	2.89685495	2.76547658
H	-3.21512317	2.81509139	3.81959450
C	-2.10688237	1.93298894	2.20557726
H	-1.72666402	1.10815790	2.80822476
C	-1.79469640	2.09005789	0.85435618
C	4.49355481	-0.13306773	-2.29310147
H	5.10032814	0.77375929	-2.41251989
H	5.14330633	-0.98065731	-2.03721135
H	3.97579810	-0.35033886	-3.23210229
C	-2.36182125	-3.82398336	-2.29434181
H	-1.87618696	-4.80057970	-2.41778409
H	-3.41943401	-3.96793449	-2.03595191
H	-2.29622653	-3.26393769	-3.23191125
C	-2.13062782	3.95860974	-2.29295789
H	-3.21911290	4.02435082	-2.41829206
H	-1.72888402	4.94702182	-2.03283703
H	-1.67596360	3.62366491	-3.23001576

[BIMMeP]$^{+}$

P	-0.31672737	0.11721850	-0.52684333
N	0.03248206	0.01820091	2.43634927
N	-2.95743029	-1.88073804	1.69780691
N	-1.60634717	-0.71345248	0.28898817
N	-0.06218861	3.50252755	1.56535425
N	-0.11728845	1.68484877	0.19877136
N	3.06876362	-1.45679018	1.01042464
N	1.18850456	-0.81156574	0.03508817
C	-0.76008964	-1.17846918	2.63562420
H	-1.24942259	-1.23585312	3.62466793
H	-0.09361387	-2.05608090	2.56834819
C	-0.58056726	1.31683339	2.65413502
H	-0.28069619	1.81300556	3.59473710
H	-1.67159777	1.16512690	2.70905803
C	1.46176650	-0.07740331	2.43296697
H	1.87633427	-0.60754677	3.31403171
H	1.89010248	0.94025973	2.45824717
C	-1.81453530	-1.27216979	1.57726578
C	-3.58992702	-1.76883691	0.46021341
C	-4.84449027	-2.24417137	0.06263563
H	-5.47041654	-2.79735161	0.76355562
C	-5.25231790	-1.98233188	-1.24358692
H	-6.22482628	-2.33866770	-1.58583047
C	-4.43522848	-1.25993403	-2.13381995
H	-4.78968705	-1.06818412	-3.14762053
C	-3.18259514	-0.77243316	-1.75211925
H	-2.56975115	-0.20180393	-2.45147143
C	-2.77738205	-1.04907642	-0.44575562

C	-0.24998467	2.21650744	1.50815441
C	0.19320093	3.91510248	0.25681353
C	0.45800867	5.20073874	-0.22725178
H	0.47163851	6.05268857	0.45328832
C	0.69265489	5.34327382	-1.59349418
H	0.89774450	6.33270594	-2.00440852
C	0.66629651	4.23364911	-2.45920070
H	0.85093499	4.38304328	-3.52402973
C	0.40704844	2.94210772	-1.99237704
H	0.38773772	2.09393748	-2.67813943
C	0.16841057	2.80930967	-0.62421518
C	1.91995365	-0.76743446	1.17674209
C	3.10475246	-1.97252586	-0.29035554
C	4.06139837	-2.74782452	-0.94807374
H	4.98709868	-3.06168688	-0.46535881
C	3.77248374	-3.10382898	-2.26395438
H	4.48802008	-3.70976797	-2.82070950
C	2.57805304	-2.69893953	-2.89210844
H	2.39200786	-3.00208240	-3.92301292
C	1.62555815	-1.92356385	-2.23323482
H	0.70374883	-1.61733465	-2.72684202
C	1.91195332	-1.56197167	-0.91394978
C	4.14501231	-1.63185217	1.98561843
H	4.37505683	-2.70044552	2.08497726
H	5.04079010	-1.09202834	1.65007581
H	3.83763432	-1.23995836	2.95957390

[BIMMePMe]$^{2+}$

N	0.01160711	0.02992961	2.06898813
N	-2.42403945	-2.58310278	1.72265262
N	-1.49537456	-1.04978419	0.30836747
N	-0.98816462	3.43582618	1.59333886
N	-0.39403537	1.72282419	0.20234034
N	3.41633991	-0.70269893	1.05233565
N	1.44348159	-0.62162014	0.03549515
C	-0.39102209	-1.33268087	2.50262771
H	-0.72160655	-1.35392119	3.55218653
H	0.47429877	-2.00866025	2.40140218
C	-0.90156312	1.10703042	2.53717311
H	-0.63920693	1.47429547	3.54087234
H	-1.92194121	0.69229291	2.57686661
C	1.43733933	0.34211942	2.29328046
H	1.78633623	-0.02016586	3.27333474
H	1.57178619	1.43699710	2.26456724
C	-1.48812321	-1.71237350	1.57407586
C	-3.15444120	-2.55921907	0.52968235
C	-4.29696858	-3.29848293	0.21414334
H	-4.69402565	-4.02115383	0.92770300
C	-4.90019178	-3.06530585	-1.01937704
H	-5.79442002	-3.62363565	-1.29831648
C	-4.38564351	-2.10372231	-1.90485092
H	-4.89421394	-1.92418428	-2.85300996
C	-3.24538599	-1.35026888	-1.60409770
H	-2.90892230	-0.59406475	-2.30944435
C	-2.62106769	-1.61202599	-0.38446413
C	-0.77667770	2.16901469	1.50586328
C	-0.76094780	3.94483516	0.31008634
C	-0.83982931	5.27708668	-0.10243624
H	-1.13918764	6.05042571	0.60571787
C	-0.52297270	5.56636897	-1.42752617
H	-0.57751198	6.59514283	-1.78504921
C	-0.12205908	4.55091130	-2.31094796
H	0.13621642	4.80831573	-3.33904528
C	-0.03301874	3.21154610	-1.91420784
H	0.30258939	2.46952978	-2.63439974
C	-0.38261316	2.91811925	-0.59579554
C	2.14510596	-0.31477491	1.16075659
C	3.58517151	-1.31542981	-0.19986611
C	4.71756690	-1.90858295	-0.75841458
H	5.67767129	-1.92361953	-0.24186902
C	4.55855775	-2.49525500	-2.01063305
H	5.41312326	-2.97339201	-2.49047538
C	3.31001505	-2.49871525	-2.66009444

H	3.21731251	-2.99057430	-3.62918934
C	2.17879296	-1.90525019	-2.09983244
H	1.22918185	-1.95553666	-2.62489204
C	2.33330496	-1.28386288	-0.85691588
C	4.48287701	-0.53698145	2.04738185
H	4.88276295	-1.52202004	2.32035095
H	5.28187565	0.08367414	1.62136312
H	4.08795368	-0.04348909	2.94111825
P	-0.25797980	0.04512008	-0.13485726
C	-0.37137772	0.03004722	-1.94830015
H	-0.60416099	-0.98195425	-2.29898000
H	-1.18051246	0.70735239	-2.24981420
H	0.56662779	0.37704258	-2.39663053

[BIMP]

N	0.00093581	0.00140662	2.52876168
N	-3.16620507	1.42748416	1.53364857
N	-1.41699629	0.77944905	0.23309850
N	2.82036677	2.02871522	1.53224337
N	1.38318862	0.83863893	0.23249110
N	0.34696786	-3.45458558	1.53410048
N	0.03443939	-1.61582153	0.23317572
C	-1.43808789	0.00579480	2.64120769
H	-1.82540071	0.44191449	3.58184822
H	-1.78643058	-1.04093158	2.61557050
C	0.72443421	1.24542362	2.64048987
H	1.29612007	1.36300192	3.58090023
H	-0.00766472	2.07064515	2.61485695
C	0.71665536	-1.24707791	2.64075344
H	0.53350435	-1.80037550	3.58167823
H	1.79730103	-1.02547688	2.61397797
C	-2.04405792	0.75673493	1.49494672
C	-3.34922753	1.93008460	0.24847300
C	-4.38854864	2.72015732	-0.25703108
H	-5.21531566	3.01785412	0.38934961
C	-4.32519634	3.10265751	-1.59585329
H	-5.12137920	3.71744839	-2.01918248
C	-3.24992308	2.71136870	-2.41704016
H	-3.23084579	3.02999831	-3.46068568
C	-2.20180194	1.92730725	-1.92929516
H	-1.37110512	1.63520560	-2.57311315
C	-2.27500959	1.54216766	-0.58878007
C	1.67758120	1.39371976	1.49392720
C	3.34728808	1.93403772	0.24725534
C	4.55216139	2.43657602	-0.25842297
H	5.22408126	3.00329937	0.38758461
C	4.85176622	2.18850707	-1.59687832
H	5.78309250	2.56855058	-2.02029269
C	3.97428545	1.45353384	-2.41755938
H	4.24075721	1.27607498	-3.46091295
C	2.77016975	0.94044015	-1.92965752
H	2.10114572	0.36747728	-2.57309339
C	2.47331217	1.19822713	-0.58949368
C	0.36795242	-2.14742282	1.49498037
C	0.00185144	-3.86446368	0.24930509
C	-0.16458448	-5.15956304	-0.25564546
H	-0.00954384	-6.02436616	0.39092673
C	-0.52874630	-5.29595812	-1.59412621
H	-0.66462130	-6.29285461	-2.01699486
C	-0.72676347	-4.16913651	-2.41555507
H	-1.01315312	-4.31195821	-3.45894590
C	-0.56990086	-2.86942257	-1.92838022
H	-0.73159781	-2.00402349	-2.57244960
C	-0.19875155	-2.74024260	-0.58816347
P	0.00006849	0.00072020	-0.47535989

[BIMPMe]$^{+}$

N	0.00031866	-0.00033253	2.14840792
N	-1.61088386	-3.15097300	1.56248712
N	-0.99489959	-1.38890497	0.25079417
N	-1.92349662	2.96977639	1.56327074
N	-0.70499417	1.55592420	0.25131534
N	3.53445473	0.18009107	1.56288478
N	1.70063841	-0.16786643	0.25103158

C	-0.04331491	-1.43326441	2.52121633
H	-0.43614261	-1.58999085	3.53702079
H	0.98202457	-1.83501264	2.48081211
C	-1.21867609	0.75370476	2.52172691
H	-1.15754492	1.17213043	3.53755696
H	-2.07917088	0.06651806	2.48150900
C	1.26301510	0.67823565	2.52145123
H	1.59502476	0.41624420	3.53725707
H	1.09839782	1.76710710	2.48108064
C	-0.91478218	-2.06336643	1.49383918
C	-2.22472391	-3.27053246	0.31307299
C	-3.10950841	-4.26435394	-0.11459939
H	-3.36347224	-5.08968901	0.55119532
C	-3.64743569	-4.15163750	-1.39377849
H	-4.34108175	-4.91020305	-1.75827867
C	-3.32252328	-3.06200282	-2.21927815
H	-3.77563798	-2.98661719	-3.20872868
C	-2.44194350	-2.05702576	-1.80809181
H	-2.24319696	-1.21936915	-2.47188881
C	-1.87630744	-2.18730302	-0.53793141
C	-1.32906280	1.82346682	1.49446787
C	-1.72067920	3.56126731	0.31382383
C	-2.13985588	4.82411989	-0.11379748
H	-2.72776527	5.45643996	0.55215470
C	-1.77411211	5.23364895	-1.39321129
H	-2.08503075	6.21338854	-1.75772064
C	-0.99278173	4.40782170	-2.21896883
H	-0.70157706	4.76258376	-3.20859094
C	-0.56177336	3.14305626	-1.80779373
H	0.06441980	2.55231178	-2.47166291
C	-0.95668906	2.71825522	-0.53742348
C	2.24451309	0.23868226	1.49416449
C	3.94513107	-0.29112857	0.31332145
C	5.24834154	-0.55952253	-0.11443844
H	6.08994493	-0.36678041	0.55152616
C	5.42007167	-1.08060245	-1.39403826
H	6.42397801	-1.30114695	-1.75867649
C	4.31417796	-1.34383925	-2.21988781
H	4.47572969	-1.77291316	-3.20974068
C	3.00339071	-1.08475880	-1.80855791
H	2.17870012	-1.33103478	-2.47266519
C	2.83300027	-0.53092850	-0.53792675
P	0.00036011	-0.00018899	-0.06766679
C	0.00046195	0.00029137	-1.88996475
H	0.09606156	-1.02759676	-2.25791304
H	-0.93756136	0.43160299	-2.25753916
H	0.84293330	0.59715651	-2.25742521

[Me]$^{+}$

C	-0.00000000	0.00011223	0.00000000
H	-0.14024884	1.09258160	0.00000000
H	-0.87575455	-0.66802849	-0.00000000
H	1.01600339	-0.42522648	0.00000000

Coordinates of optimized structures with MeCN as solvent model.

[Me]+

1 1

C	-0.00000000	-0.00005162	0.00000000
H	-0.56509083	0.93912743	-0.00000000
H	-0.53104044	-0.95902451	0.00000000
H	1.09613127	0.02020681	0.00000000

[BIMPMe]$^{+}$

N	-0.00306964	-0.00108155	2.13366801
N	0.24011110	3.53999769	1.56245836
N	0.37885023	1.67517342	0.26187644
N	2.94438009	-1.97955655	1.56495049
N	1.26188243	-1.16682236	0.26208468
N	-3.19053838	-1.56100075	1.56039017
N	-1.64300734	-0.51087464	0.25997072
C	-0.51602093	1.33582745	2.52040961
H	-0.20836977	1.61268814	3.53823355
H	-1.61594809	1.31509960	2.48452231
C	1.41015390	-0.22604793	2.52308785

H	1.49351324	-0.63278426	3.54038453
H	1.94231171	0.73690875	2.49006373
C	-0.90470585	-1.11330699	2.52018471
H	-1.29946241	-0.98481241	3.53752212
H	-0.33682439	-2.05559576	2.48495075
C	0.03588517	2.26009052	1.49593571
C	0.75906369	3.88692490	0.31217288
C	1.17715985	5.14769764	-0.12510308
H	1.08441417	6.01346791	0.53187169
C	1.71598075	5.24941684	-1.40592492
H	2.05105173	6.21904550	-1.77693791
C	1.84863006	4.11381115	-2.22408684
H	2.29134221	4.21569429	-3.21588537
C	1.43925048	2.84534287	-1.80258810
H	1.58429109	1.99235604	-2.45961874
C	0.87020614	2.74884003	-0.53103793
C	1.93686947	-1.16423890	1.49789753
C	2.98967988	-2.59925523	0.31327569
C	3.87554975	-3.58890121	-0.12427016
H	4.67072030	-3.94156924	0.53383017
C	3.69862583	-4.10348303	-1.40687856
H	4.37325309	-4.87625735	-1.77809942
C	2.65021372	-3.65039094	-2.22666116
H	2.52055902	-4.08231928	-3.21998981
C	1.75351557	-2.66430728	-1.80497381
H	0.94361923	-2.36308496	-2.46347126
C	1.94987624	-2.12619860	-0.53141987
C	-1.97995152	-1.09798715	1.49460958
C	-3.74893863	-1.28687834	0.30907266
C	-5.04956858	-1.55530259	-0.12889188
H	-5.75365829	-2.06729550	0.52828611
C	-5.40598307	-1.14098063	-1.41047640
H	-6.41310681	-1.33550833	-1.78191547
C	-4.48790784	-0.45977505	-2.22876360
H	-4.79659040	-0.12831461	-3.22117697
C	-3.18483381	-0.18021288	-1.80667304
H	-2.51796007	0.37070476	-2.46397250
C	-2.81781563	-0.62322626	-0.53421012
P	-0.00125621	-0.00100172	-0.05125538
C	-0.00050472	-0.00096546	-1.86877935
H	-0.49644415	0.90298626	-2.23824108
H	1.03076541	-0.02349435	-2.23728091
H	-0.53547227	-0.88269387	-2.23748131
[BIMP]			
N	0.00014675	-0.00108619	2.50901397
N	-2.18811724	-2.71955210	1.53786932
N	-1.11188266	-1.18552351	0.25451096
N	-1.26202807	3.25296094	1.53857601
N	-0.47041536	1.55491640	0.25455438
N	3.44936929	-0.53362689	1.53796998
N	1.58269653	-0.37074720	0.25430705
C	-0.40370046	-1.37879203	2.66862385
H	-0.94586178	-1.58805695	3.60934595
H	0.50219566	-2.00737628	2.68377914
C	-0.99123908	1.03733782	2.66878113
H	-0.90110866	1.61172872	3.60933511
H	-1.98831856	0.56661895	2.68473351
C	1.39505390	0.33842700	2.66875774
H	1.84773824	-0.02658989	3.60925426
H	1.48550300	1.43725040	2.68475870
C	-1.26385368	-1.78968735	1.51308243
C	-2.69551713	-2.78164655	0.24160408
C	-3.70316381	-3.60161384	-0.28276216
H	-4.20968838	-4.33098906	0.35159127
C	-4.02950070	-3.45287027	-1.63088741
H	-4.80923763	-4.07859701	-2.06864735
C	-3.37024053	-2.50752822	-2.44196387
H	-3.64987618	-2.41692045	-3.49293935
C	-2.36634931	-1.67809864	-1.93450961
H	-1.86576067	-0.94777875	-2.57126146
C	-2.04116860	-1.83614813	-0.58498592
C	-0.91791529	1.98788327	1.51329535

C	-1.06239931	3.72405708	0.24252709
C	-1.26981749	5.00676160	-0.28120490
H	-1.64879062	5.80948538	0.35359526
C	-0.97817863	5.21589235	-1.62925428
H	-1.13110887	6.20406830	-2.06659369
C	-0.48843823	4.17304538	-2.44087000
H	-0.27049472	4.37058765	-3.49180021
C	-0.27115969	2.88880126	-1.93410890
H	0.11132353	2.09062677	-2.57133595
C	-0.57009347	2.68530384	-0.58455586
C	2.18156492	-0.19968084	1.51297271
C	3.75748305	-0.94180826	0.24183526
C	4.97219112	-1.40288784	-0.28210828
H	5.85704116	-1.47554670	0.35249864
C	5.00743032	-1.75990135	-1.63017768
H	5.93980607	-2.12103781	-2.06766951
C	3.85913388	-1.66335648	-2.44151593
H	3.92110419	-1.95102111	-3.49240203
C	2.63809715	-1.21022822	-1.93448161
H	1.75535940	-1.14324904	-2.57146342
C	2.61156833	-0.84919008	-0.58503711
P	0.00020444	-0.00060149	-0.44471515

[BIMMePMe]$^{2+}$

N	0.00694412	0.00264167	2.04759429
N	-2.42694380	-2.61722863	1.70026758
N	-1.49745224	-1.07076891	0.30971411
N	-1.08676769	3.39634804	1.59388257
N	-0.40404369	1.71050542	0.22087291
N	3.42745796	-0.66503881	1.06272816
N	1.45422038	-0.63148418	0.05008342
C	-0.38419324	-1.36618392	2.47695226
H	-0.69726641	-1.38645601	3.52953242
H	0.47921416	-2.03854411	2.35874620
C	-0.91981307	1.06208465	2.52951049
H	-0.64659255	1.41799620	3.53208759
H	-1.93516538	0.63962370	2.57555905
C	1.42982612	0.32124775	2.30585261
H	1.75325749	-0.05135673	3.28858245
H	1.57041353	1.41347212	2.28972791
C	-1.48438395	-1.74242801	1.55310789
C	-3.15659325	-2.57015923	0.50800584
C	-4.30065285	-3.30003642	0.17339978
H	-4.70531543	-4.03392445	0.87129023
C	-4.89684345	-3.04819525	-1.06049202
H	-5.79077182	-3.60108121	-1.35203133
C	-4.37123646	-2.07785207	-1.93096818
H	-4.86771015	-1.88555255	-2.88295795
C	-3.23014065	-1.33559563	-1.61139475
H	-2.87539321	-0.57734746	-2.30402431
C	-2.61589579	-1.61197312	-0.38947897
C	-0.82494914	2.13189445	1.50341977
C	-0.83958846	3.91128069	0.31690218
C	-0.94084100	5.23953630	-0.10641278
H	-1.28112944	6.01045309	0.58586822
C	-0.58582525	5.53371212	-1.42134737
H	-0.65436749	6.56033043	-1.78348415
C	-0.12356439	4.52679109	-2.28606719
H	0.16814166	4.78607765	-3.30462422
C	-0.01216395	3.19389318	-1.87862175
H	0.37705126	2.45438658	-2.57289555
C	-0.40187349	2.89498052	-0.57278587
C	2.15235759	-0.31667149	1.17767355
C	3.60881574	-1.26012651	-0.19418436
C	4.75556412	-1.81637702	-0.75809517
H	5.71198071	-1.80963869	-0.23645587
C	4.61212609	-2.39335152	-2.01702602
H	5.47953670	-2.84253354	-2.50091764
C	3.36530415	-2.42269012	-2.66679978
H	3.28301065	-2.90296136	-3.64208263
C	2.21847887	-1.86754014	-2.09906185
H	1.26975933	-1.93597754	-2.62184771
C	2.35898417	-1.25744299	-0.85101389

C	4.48688793	-0.46974772	2.05652263
H	4.90688671	-1.44500071	2.32868112
H	5.26422560	0.17158233	1.62459259
H	4.07266120	0.01464497	2.94471848
P	-0.22359155	0.01985300	-0.11580053
C	-0.34876122	0.01210771	-1.92550913
H	-0.56613425	-1.00194761	-2.27746093
H	-1.16619112	0.67809717	-2.22450649
H	0.58371517	0.36609667	-2.37761856

[BIMMeP]$^{+}$

P	-0.28313601	0.04416524	-0.48701484
N	0.06136025	-0.01700266	2.41297931
N	-2.54965590	-2.42917392	1.69383884
N	-1.41952138	-1.02552686	0.31194221
N	-0.78924359	3.40951154	1.61243147
N	-0.42634652	1.62910013	0.25016984
N	3.32254706	-0.88272421	0.99535395
N	1.35687285	-0.56056294	0.03199772
C	-0.52707095	-1.31897117	2.65465358
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H	-1.78201856	0.83979732	2.83389512
C	1.49507990	0.10475898	2.45770901
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H	1.77404389	1.16794812	2.54658982
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C	-3.17009777	-2.43166499	0.44501442
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H	-5.60592073	-3.48116855	-1.66278494
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H	-4.39309915	-1.96195996	-3.19648428
C	-2.90575694	-1.37264077	-1.76117751
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H	-0.10249630	2.11618594	-2.63132279
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C	2.07045081	-0.43738368	1.18441830
C	3.45914382	-1.31069750	-0.32929720
C	4.55014058	-1.85027298	-1.01196967
H	5.51442705	-2.00442536	-0.52873889
C	4.34260775	-2.18066604	-2.35013797
H	5.16527715	-2.60496332	-2.92654105
C	3.09653924	-1.97665524	-2.97525355
H	2.97702720	-2.24786583	-4.02473151
C	2.00810312	-1.43759198	-2.28986325
H	1.04865703	-1.28353232	-2.78217065
C	2.21381638	-1.10475362	-0.94905509
C	4.40688477	-0.89827007	1.97819771
H	4.86313182	-1.89488848	1.98940549
H	5.15770649	-0.14562490	1.70649018
H	4.01144769	-0.67138429	2.97154820

[BIMMe$_2$PMe]$^{3+}$

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H	-1.48851528	-0.93770351	-3.26705165
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C	-0.22543568	2.27038184	-1.60663941
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H	-2.33432895	6.46176852	1.29735053
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C	-1.02191520	2.93732401	0.40009564
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C	-1.47973204	-2.43848406	2.24056289
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C	-1.78814483	-2.02590073	0.94393312
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C	5.11698624	-1.14961193	0.48897145
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C	5.43432072	-0.52220599	1.69062096
H	6.43682353	-0.63465666	2.10338723
C	4.49227785	0.27088542	2.36957842
H	4.78274065	0.77079776	3.29371509
C	3.19407165	0.45623403	1.89298168
H	2.50908945	1.10393467	2.43117064
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C	3.90531882	-2.24186006	-2.17897718
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H	3.25026144	-2.38026745	-3.04297780
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H	-1.02264516	0.30690402	2.36298778
H	0.60985472	-0.42311249	2.43345223
N	-2.87223034	-2.08659094	-1.05255913
C	-3.83904491	-2.44188757	-2.09558741
H	-3.53400093	-1.99587421	-3.04610381
H	-3.86614352	-3.53279046	-2.19376572
H	-4.82692876	-2.06056301	-1.81090379

$[BIMMe_2P]^{2+}$

P	-0.03063319	0.28866586	0.54491945
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N	-0.88300771	3.36442546	-1.83894023
N	-0.51257721	1.70919427	-0.32938895
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N	-1.09974006	-1.06603319	0.00780964
N	3.33666613	-1.06153368	-1.11812026
N	1.59682396	-0.18349472	-0.07252067
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H	-0.27649800	1.50719549	-3.69744487
H	1.24505061	1.49330564	-2.79583680
C	-1.29811224	-0.71320618	-2.47317077
H	-1.35327145	-1.43334558	-3.30777709
H	-2.03430992	0.07663006	-2.69475536
C	1.16049380	-0.98418358	-2.42153456

H	1.73660501	-0.82732532	-3.35010042
H	0.83947386	-2.03883131	-2.43374631
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C	-1.28411296	3.80790494	-0.57722070
C	-1.83896045	5.03818443	-0.20617347
H	-2.00732230	5.81681237	-0.95142839
C	-2.16172232	5.22593429	1.13763746
H	-2.59378758	6.17456063	1.45999084
C	-1.94071054	4.21286999	2.09064465
H	-2.20465481	4.39272864	3.13386031
C	-1.39225351	2.97673173	1.73649932
H	-1.23047270	2.20117768	2.48579420
C	-1.06636703	2.80172157	0.39147874
C	-1.67584836	-1.37976457	-1.18790820
C	-2.62825122	-2.69787539	0.34017405
C	-3.39879333	-3.64391074	1.01677465
H	-4.12571028	-4.27099548	0.50168548
C	-3.18915393	-3.74448251	2.39098271
H	-3.76771587	-4.46859224	2.96525162
C	-2.24862798	-2.93270420	3.05504889
H	-2.11553460	-3.04418178	4.13154779
C	-1.47868026	-1.98903140	2.37533128
H	-0.75262466	-1.36840592	2.89904250
C	-1.69073964	-1.88472126	0.99961696
C	2.03741474	-0.75733980	-1.22913347
C	3.78824745	-0.69025250	0.15371116
C	5.04711997	-0.79723827	0.74552813
H	5.89609831	-1.23336601	0.22018609
C	5.16142169	-0.31599031	2.04844684
H	6.12511950	-0.37700538	2.55483545
C	4.06173781	0.24624377	2.72609691
H	4.19457804	0.61184836	3.74475612
C	2.80455666	0.35163973	2.13146528
H	1.96200774	0.79054936	2.66450538
C	2.68806297	-0.13370993	0.82775111
C	-3.42969273	-2.95769737	-2.04351889
H	-3.27112682	-4.04257861	-2.04113062
H	-4.48035611	-2.73207230	-1.82339589
H	-3.17454511	-2.55338061	-3.02607280
C	4.17776982	-1.71009654	-2.12636160
H	5.08386573	-1.11063558	-2.27217083
H	4.44473694	-2.71682926	-1.78133515
H	3.63683702	-1.78384065	-3.07298238

Xray

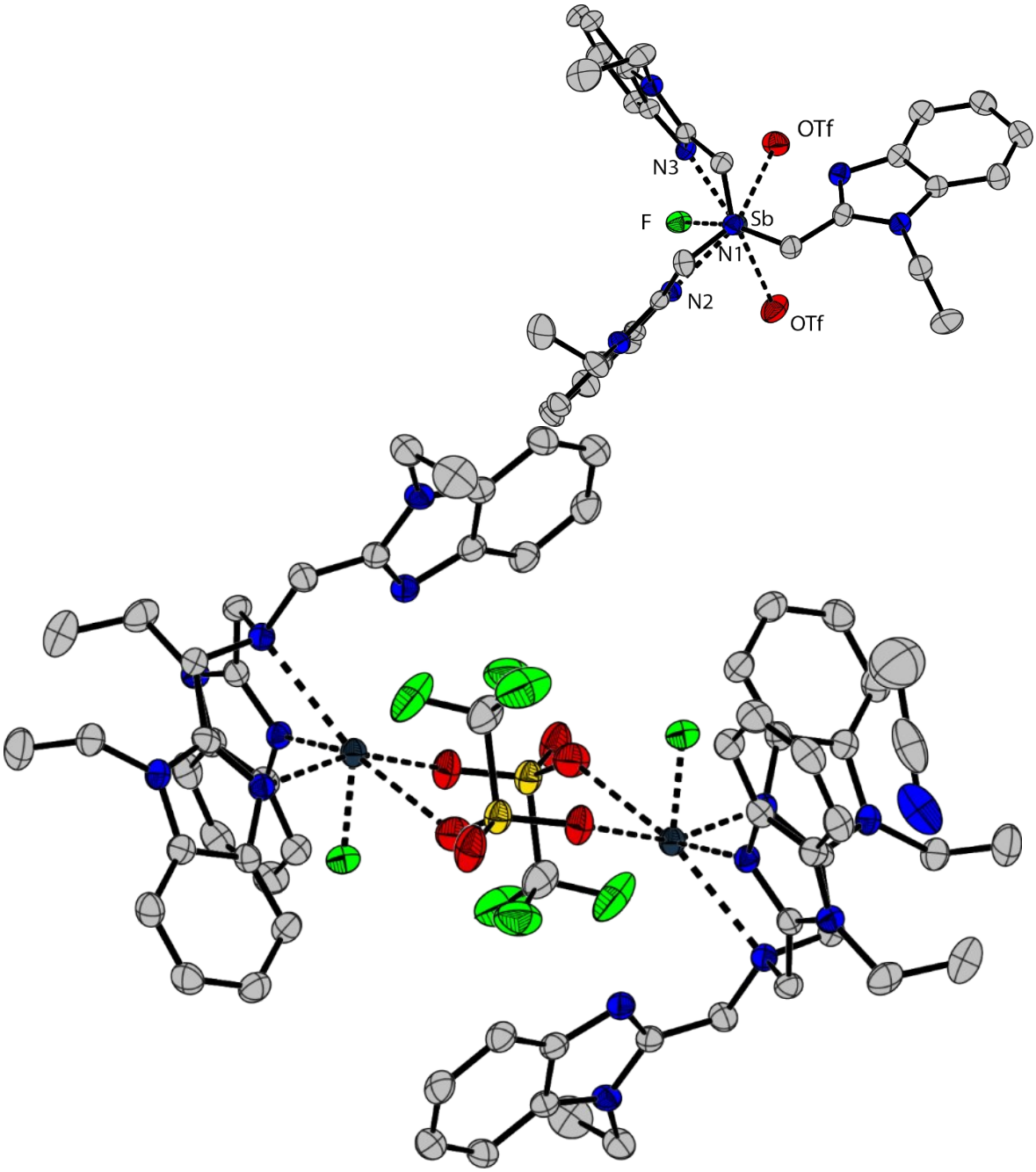

Figure S2: Structure of [{SbF(BIMEt$_3$)(OTf)}$_2$][OTf]$_4$ (*left*), Thermal ellipsoids are shown at a 50% probability level. Hydrogen atoms and solvent molecules are omitted for clarity, for the triflate anions the coordinating oxygen atoms are shown. Interatomic distances and angles are summarized in Table 1.

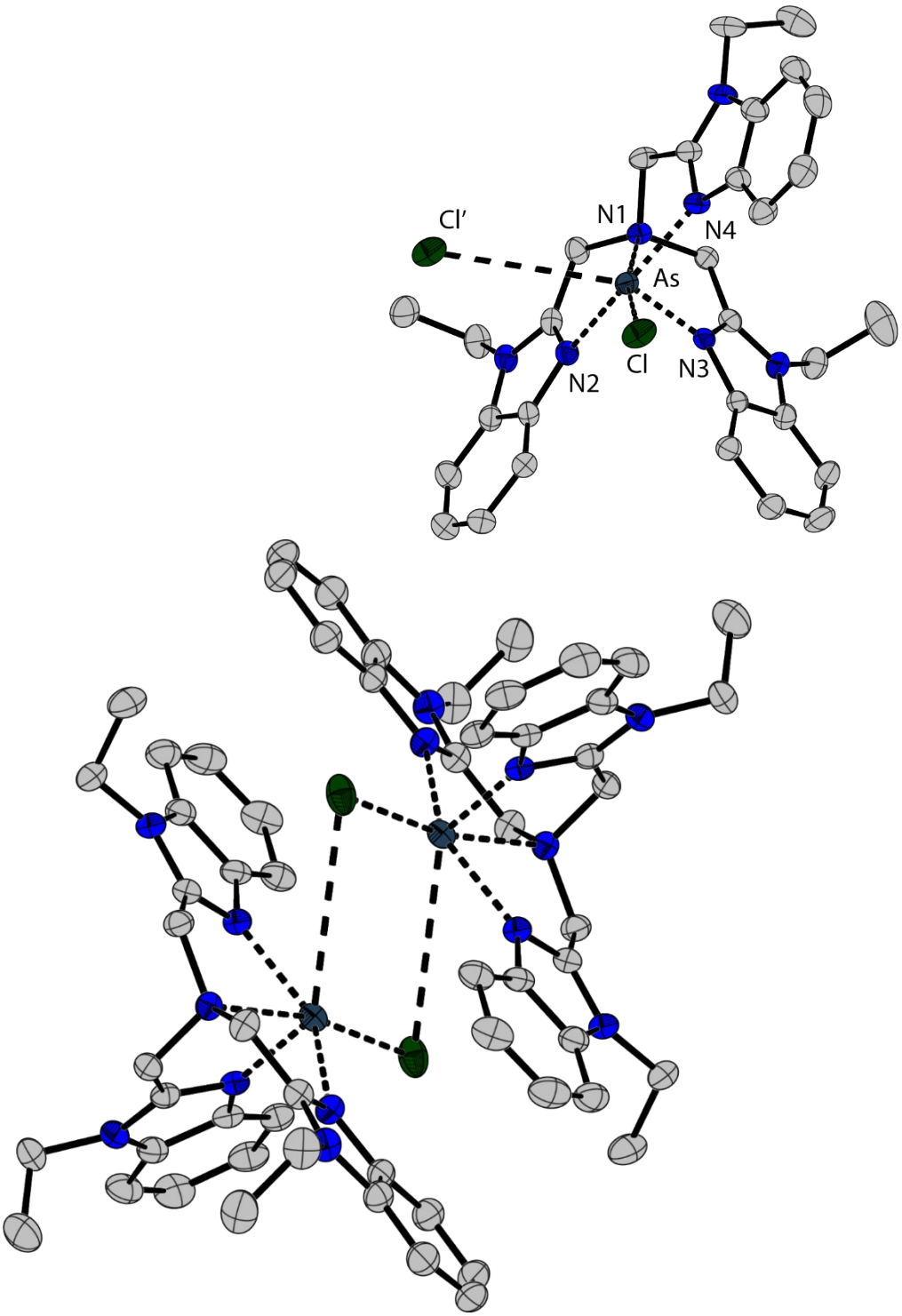

Figure S3: Structure of $[\{AsCl(BIMEt_3)(OTf)\}_2][OTf]_4$ (*left*), Thermal ellipsoids are shown at a 50% probability level. Hydrogen atoms, triflate anions and solvent molecules are omitted for clarity. Interatomic distances and angles are summarized in Table 1.

Table S2: Crystal data and structure refinement for $[BIMEt_3AsCl][OTf]_2$.

Identification code	CCDC 1578584
Empirical formula	$C_{36}H_{36}AsClF_6N_9O_6S_2$
Formula weight	979.23
Temperature/K	150.0
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	14.2067(6)
b/Å	15.9799(8)
c/Å	18.6556(10)
α/°	90
β/°	94.050(2)
γ/°	90
Volume/Å^3	4224.6(4)
Z	4
ρ_{calc}g/cm^3	1.540
μ/mm^{-1}	1.049
F(000)	1996.0
Crystal size/mm^3	0.24 × 0.2 × 0.18
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.548 to 63.11
Index ranges	-18 ≤ h ≤ 20, -23 ≤ k ≤ 23, -27 ≤ l ≤ 27
Reflections collected	210673
Independent reflections	13753 [R_{int} = 0.0748, R_{sigma} = 0.0464]
Data/restraints/parameters	13753/0/527
Goodness-of-fit on F^2	1.090
Final R indexes [I>=2σ (I)]	R_1 = 0.0512, wR_2 = 0.1096
Final R indexes [all data]	R_1 = 0.1031, wR_2 = 0.1381
Largest diff. peak/hole / e Å^{-3}	0.81/-0.68

Table S3: Crystal data and structure refinement for [BIMP].

Identification code	CCDC 1578585
Empirical formula	$C_{50}H_{39}N_{15}P_2$
Formula weight	911.90
Temperature/K	140.0
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	13.0553(5)
b/Å	25.1646(12)
c/Å	14.6359(6)
α/°	90
β/°	114.6194(15)
γ/°	90
Volume/Å^3	4371.2(3)
Z	4
ρ_{calc}g/cm^3	1.386
μ/mm^{-1}	0.157
F(000)	1896.0
Crystal size/mm^3	0.29 × 0.23 × 0.2
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.742 to 56.646
Index ranges	-17 ≤ h ≤ 17, -33 ≤ k ≤ 33, -19 ≤ l ≤ 19
Reflections collected	206509
Independent reflections	10847 [R_{int} = 0.0485, R_{sigma} = 0.0152]
Data/restraints/parameters	10847/0/605
Goodness-of-fit on F^2	1.094
Final R indexes [I>=2σ (I)]	R_1 = 0.0385, wR_2 = 0.0899
Final R indexes [all data]	R_1 = 0.0495, wR_2 = 0.0988
Largest diff. peak/hole / e Å^{-3}	0.32/-0.40

Table S4: Crystal data and structure refinement for $[BIMEt_3Sb][OTf]_3$.

Identification code	CCDC 1578586
Empirical formula	$C_{76}H_{81}F_{18}N_{19}O_{18}S_6Sb_2$
Formula weight	2326.49
Temperature/K	150.01
Crystal system	triclinic
Space group	P-1
a/Å	12.726(5)
b/Å	18.899(8)
c/Å	20.823(8)
α/°	102.659(14)
β/°	97.475(14)
γ/°	99.315(14)
Volume/Å^3	4750(3)
Z	2
ρ_{calc}g/cm^3	1.6264
μ/mm^{-1}	0.810
F(000)	2348.5
Crystal size/mm^3	0.29 × 0.28 × 0.13
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	5.44 to 55
Index ranges	-17 ≤ h ≤ 18, -26 ≤ k ≤ 26, -29 ≤ l ≤ 29
Reflections collected	133890
Independent reflections	21371 [R_{int} = 0.0637, R_{sigma} = 0.0576]
Data/restraints/parameters	21371/6/1263
Goodness-of-fit on F^2	1.063
Final R indexes [I>=2σ (I)]	R_1 = 0.0368, wR_2 = 0.0846
Final R indexes [all data]	R_1 = 0.0582, wR_2 = 0.0993
Largest diff. peak/hole / e Å^{-3}	2.19/-1.25

Table S5: Crystal data and structure refinement for $[BIMEt_3P][OTf]_3$.

Identification code	1578587
Empirical formula	$C_{39}H_{42}F_9N_{10}O_9PS_3$
Formula weight	1092.99
Temperature/K	150.0
Crystal system	triclinic
Space group	P-1
a/Å	10.8599(7)
b/Å	10.9646(8)
c/Å	20.3805(14)
α/°	81.217(2)
β/°	83.234(2)
γ/°	89.295(2)
Volume/Å^3	2381.6(3)
Z	2
ρ_{calc}g/cm^3	1.5240
μ/mm^{-1}	0.288
F(000)	1125.7
Crystal size/mm^3	0.26 × 0.2 × 0.06
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	5.64 to 61.22
Index ranges	-15 ≤ h ≤ 14, -15 ≤ k ≤ 15, -29 ≤ l ≤ 29
Reflections collected	112259
Independent reflections	14440 [R_{int} = 0.0634, R_{sigma} = 0.0474]
Data/restraints/parameters	14440/0/646
Goodness-of-fit on F^2	1.069
Final R indexes [I>=2σ (I)]	R_1 = 0.0539, wR_2 = 0.1264
Final R indexes [all data]	R_1 = 0.0940, wR_2 = 0.1480
Largest diff. peak/hole / e Å^{-3}	1.21/-1.17

Table S6: Crystal data and structure refinement for $[BIMEt_3As][OTf]_3$.

Identification code	CCDC 1581022
Empirical formula	$C_{37}H_{39}AsF_9N_9O_9S_3$
Formula weight	1095.87
Temperature/K	173.15
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	14.0065(3)
b/Å	15.9167(3)
c/Å	21.8331(5)
α/°	90
β/°	107.9657(13)
γ/°	90
Volume/Å^3	4630.08(17)
Z	4
ρ_{calc}g/cm^3	1.572
μ/mm^{-1}	3.138
F(000)	2232.0
Crystal size/mm^3	0.57 × 0.259 × 0.223
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	6.634 to 136.478
Index ranges	-14 ≤ h ≤ 16, -19 ≤ k ≤ 19, -26 ≤ l ≤ 25
Reflections collected	25884
Independent reflections	8479 [R_{int} = 0.0804, R_{sigma} = 0.0654]
Data/restraints/parameters	8479/0/615
Goodness-of-fit on F^2	1.057
Final R indexes [I>=2σ (I)]	R_1 = 0.0898, wR_2 = 0.2548
Final R indexes [all data]	R_1 = 0.0989, wR_2 = 0.2635
Largest diff. peak/hole / e Å^{-3}	3.21/-2.02

Table S7: Crystal data and structure refinement for $[BIMEt_3SbF][OTf]_2$.

Identification code	CCDC 1581023
Empirical formula	$C_{36}H_{39}F_7N_9O_6S_2Sb$
Formula weight	1012.63
Temperature/K	193.15
Crystal system	triclinic
Space group	P-1
a/Å	13.1877(6)
b/Å	13.3482(7)
c/Å	13.4824(7)
α/°	79.6653(7)
β/°	63.0215(6)
γ/°	84.7868(7)
Volume/Å^3	2080.63(18)
Z	2
ρ_{calc}g/cm^3	1.616
μ/mm^{-1}	0.851
F(000)	1024.0
Crystal size/mm^3	0.227 × 0.183 × 0.133
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.102 to 55.13
Index ranges	-17 ≤ h ≤ 17, -17 ≤ k ≤ 17, -17 ≤ l ≤ 17
Reflections collected	18546
Independent reflections	9603 [R_{int} = 0.0385, R_{sigma} = 0.0608]
Data/restraints/parameters	9603/0/552
Goodness-of-fit on F^2	1.039
Final R indexes [I>=2σ (I)]	R_1 = 0.0434, wR_2 = 0.1033
Final R indexes [all data]	R_1 = 0.0586, wR_2 = 0.1125
Largest diff. peak/hole / e Å^{-3}	1.21/-0.60

Table S8: Crystal data and structure refinement for $[BIMEt_3PF_2][OTf]_3$.

Identification code	CCDC 1819912
Empirical formula	$C_{37}H_{39}F_{11}N_9O_9PS_3$
Formula weight	1089.92
Temperature/K	170.02
Crystal system	triclinic
Space group	P-1
a/Å	13.753(7)
b/Å	14.060(7)
c/Å	14.321(7)
α/°	109.504(13)
β/°	98.444(13)
γ/°	111.998(9)
Volume/Å^3	2300.1(19)
Z	2
ρ_{calc}g/cm^3	1.574
μ/mm^{-1}	0.304
F(000)	1116.0
Crystal size/mm^3	0.24 × 0.14 × 0.06
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.802 to 49.424
Index ranges	-16 ≤ h ≤ 16, -16 ≤ k ≤ 16, -16 ≤ l ≤ 16
Reflections collected	55372
Independent reflections	7797 [R_{int} = 0.1024, R_{sigma} = 0.0674]
Data/restraints/parameters	7797/0/636
Goodness-of-fit on F^2	1.083
Final R indexes [I>=2σ (I)]	R_1 = 0.1889, wR_2 = 0.5278
Final R indexes [all data]	R_1 = 0.2467, wR_2 = 0.5690
Largest diff. peak/hole / e Å^{-3}	1.42/-1.01

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