Supporting Information for:

α-Cationic Arsines: Synthesis, Structure, Reactivity, and Applications

By: Jonathan W. Dube, Yiying Zheng, Walter Thiel, and Manuel Alcarazo

Georg-August Universtät Göttingen, Institut für Organische und Biomolekulare Chemie, Tammannstr. 2, 37077 Göttingen, Germany

Max-Planck-Institut für Kohlenforschung, Kaiser-Wilhelm-Platz 1, 45470 Mülheim an der Ruhr, Germany

Contents:

1) General Experimental

All manipulations were performed under an inert argon atmosphere on a Schlenk line using standard manipulations unless otherwise stated. Solvents were dried and distilled in house and stored under a positive pressure of argon. Solvents for NMR spectroscopy, $CDCl_3$, CD_2Cl_2, and CD_3CN were dried over CaH_2, distilled, and stored under an argon atmosphere over 4Å ($CDCl_3$, CD_2Cl_2) or 3Å (CD_3CN) molecular sieves. Solution ^{1}H, $^{13}C\{^{1}H\}$, $^{11}B\{^{1}H\}$, $^{19}F\{^{1}H\}$, $^{27}Al\{^{1}H\}$, $^{31}P\{^{1}H\}$ NMR spectroscopy was recorded on a Bruker AV 400 MHz spectrometer (^{1}H 400.0 MHz, $^{13}C\{^{1}H\}$ 100.5 MHz, $^{31}P\{^{1}H\}$ 161.82 MHz), or Bruker DPX 300 MHz spectrometer (^{1}H 300.0 MHz, $^{11}B\{^{1}H\}$ 96.3 MHz, $^{19}F\{^{1}H\}$ 282.2 MHz, $^{27}Al\{^{1}H\}$ 78.1 MHz) unless otherwise stated. All samples for ^{1}H spectroscopy were referenced to the residual protons in the deuterated solvent relative to $Si(CH_3)_4$, while samples for $^{13}C\{^{1}H\}$ NMR spectroscopy were referenced to the ^{13}C signal of the solvent relative to $Si(CH_3)_4$ (CH_2Cl_2: δ_H = 5.32, $^{13}C\{^{1}H\}$ δ_C = 54.0; $CDCl_3$: ^{1}H δ_H = 7.26, $^{13}C\{^{1}H\}$ δ_C = 77.16, CD_3CN: δ_H = 1.95, $^{13}C\{^{1}H\}$ δ_C = 118.3). Chemical shifts for $^{11}B\{^{1}H\}$, $^{19}F\{^{1}H\}$, $^{27}Al\{^{1}H\}$, $^{31}P\{^{1}H\}$ NMR spectroscopy were referenced internally by the instrument after locking and shimming to the deutrated solvent. Coupling constants are reported in Hz. FT-IR spectroscopy was performed on neat solid samples using the ATR mode on a Bruker ATR Diamond spectrometer with a spectral range of 4000-400 cm^{-1}. Wavenumbers are reported in inverse centimeters. Signals attributable to CO stretching frequency in the rhodium compounds are highlighted in bold font. Mass spectrometry was recorded in house in positive and negative ion modes using an Finnigan MAT 95 spectrometer for electro-spray ionization (ESI) measurements and a Bruker Apex III FT-MS (7 T magnet) for the high resolution measurements. For the high resolution measurements, the difference from the theoretical mass is reported in parenthesis. Column chromatography was performed on Merck 60 silica gel (40-63 um), while thin layer chromatography was performed using Merck silica gel 60 F254 TLC plates and visualized by UV light. Analytical measurements by gas chromatography were conducted with an Agilent 6890A device with an Agilent 5973 Mass Selective Detector.

Reagents and Handling:

Triphenylarsine, triphenylphosphine, arsenic(III) oxide, xenon difluoride, and *meta*-chloroperbenzoic acid (77%) were obtained from Sigma Aldrich and used as received. Lithium sand was obtained from Sigma Aldrich and handled carefully under argon. Trimethylsilylchloride was also obtained from Sigma Aldrich and was dried (CaH_2), distilled, and stored under argon at 4 °C. The transition metal precursors were all purchased from commercially available sources (Sigma Aldrich, Alfa Aesar, Strem Chemicals) and used as received. Aluminum trichloride was purchased from Sigma Aldrich, purified by sublimation, and stored under argon.

The synthesis and characterization of arsenic starting materials are described below and were closely adapted from literature protocols. The *N*-heterocyclic carbene, 1,3-bis(2,4,6-trimethylphenyl)imidazol-2-ylidene (IMes) was prepared by literature procedure.[1] All cationic arsine precursors: 2,3-bis(diisopropylamino)-1-chlorocyclopropenium tetrafluoroborate,[2] 2,3-bis(diisopropylamino)-1-iodocyclopropenium triflate,[3] 1-chloro-di(piperdin)formamidinium hexafluoroantimonate,[4] and 1-ethyl-4-trifluoromethyl-2-chloro-pyridinium tetrafluoroborate[5] were prepared in multi-gram quantities by following also literature procedures. The synthesis and characterization of 2,3-bis(diisopropylamino)-1-iodocyclopropenium triflate, 1-methyl-4-iodo-pyridinium trifluoromethanesulfonate, and 1-methyl-2-iodo-pyridinium trifluoromethanesulfonate are described after the arsenic compounds they are used for (**7**, **10**, and **11**, respectively).

Arsenic-containing compounds were handled using standard procedures for any toxic reagent. Any residues or glassware containing arsenic was oxidized with bleach and kept in a separate waste container.

2) Synthesis and characterization data of reported compounds

Synthesis of Arsenic Starting Materials Ph_2AsI (**1**), $Ph_2As(SiMe_3)$ (**5**), and Ph_2AsH (**12**)

Synthesis of Ph_2AsI (**1**), *via* tetraphenylarsyl oxide $Ph_2AsOAsPh_2$:
This synthetic approach was closely adapted from literature procedures.[6,7] A solution of PhMgBr (13.5 mL, 40.4 mmol, 4 equiv.; 3M in Et_2O) was diluted with an additional amount of Et_2O (10 mL) and benzene (20 mL), and cooled to 0 °C in a three-neck round bottom flask equipped with a reflux condenser. Through an open neck, under a flow of argon, was added arsenic(III) oxide (2.00 g, 10.1 mmol, 1 equiv.) as quickly as possible, resulting in a moderate heat evolution. The reaction was stirred at 0 °C for 5 minutes and then for 3 hours at room temperature, resulting in the formation of a considerable amount of white precipitate. Approximately two thirds of the solvent volume was removed *in vacuo* and the remaining filtrate was decanted from the precipitate. Ice mixed with glacial acetic acid (0.4 mL) was added to the precipitate, which was then extracted with benzene (50 mL). The organic phase was washed with dilute aqueous NaOH (~0.1M), dried with Na_2SO_4, and the volatiles were removed *in vacuo* to give a colourless oil that solidifies to a white powder shortly after dryness. The solids were washed with *n*-pentane (3 x 5 mL) and a mixture of *n*-pentane and Et_2O (1:1, 2 x 4 mL) to give tetraphenylarsyl oxide as a colourless solid after drying. The compound is a reasonably air and moisture stable solid that shows no signs of decomposition after months of storage under ambient conditions. The combined organic fractions resulting from the washing, including the initially decanted reaction mixture, were subjected to the same workup procedure as before, starting with the addition of ice and glacial acetic acid, to give a second crop of the compound.
Yield: 63%, 3.02 g, 6.36 mmol (lit. 55%, 26 g);
m.p.: 92.1-94.6 °C (lit. 92.5-93.5 °C)
^{1}H NMR (300 MHz, $CDCl_3$, δ_H): 7.30-7.38 (m, 6H), 7.47-7.54 (m, 4H);
^{13}C{^{1}H} NMR (75.6 MHz, $CDCl_3$, δ_C): 128.5, 129.3, 131.1, 146.4;
FT-IR (ν, cm^{-1}): 448, 481, 551, 668, 692, 722, 734, 748, 917, 997, 1023, 1065, 1073, 1155, 1174, 1273, 1300, 1433, 1478, 1577, 1809, 1963, 3032, 3065;
ESI-MS (m/z): 497 $[M + Na^+]^+$;
HRMS (m/z): calculated for $C_{24}H_{20}As_2Na_1O_1$ $[M + Na^+]^+$: 496.983789; found: 496.983630 (0.32 ppm).

To an argon filled Schlenk flask of tetraphenylarsyl oxide (1.00 g, 2.11 mmol) was added hydrogen iodide (0.946 g, 0.556 mL, 4.217 mmol, 57% in H_2O) and the neat reaction mixture was heated to 100 °C for 2 hours. The resulting yellow residue was dissolved in CH_2Cl_2 (10 mL), dried with Na_2SO_4, and the volatiles were removed *in vacuo* to give a viscous yellow oil (**1**) that was determined to be pure by NMR spectroscopy. The compound is indefinitely stable when stored under argon and solidifies to a low melting yellow solid when it is a suitable purity and dryness.
Yield: 95%, 1.43 g, 4.00 mmol;
^{1}H NMR (300 MHz, $CDCl_3$, δ_H): 7.33-7.41 (m, 6H), 7.64-7.71 (m, 4H);
^{13}C{^{1}H} NMR (75.6 MHz, $CDCl_3$, δ_C): 129.0, 129.9, 133.7, 137.5;
FT-IR (ν, cm^{-1}): 455, 477, 516, 571, 636, 689, 732, 856, 997, 1029, 1067, 1151, 1182, 1223, 1254, 1276, 1432, 1478, 3048;
EI-MS (m/z): 356 $[M]^+$, 229 $[M - I^-]^+$, 152 $[M - Ph - I^-]^+$;

Synthesis of $Ph_2As(TMS)$ (**5**):
This synthetic approach was closely adapted from a literature procedure.[8] To a THF solution (10 mL) of $AsPh_3$ (6.00 g, 19.6 mmol, 1 equiv.) cooled to 0 °C was added solid lithium sand (292 mg, 42.1 mmol, 2.15 equiv.) slowly over the course of five minutes, resulting in a deep red solution. The reaction mixture was allowed to stir for three hours after warming to room temperature. The solution was then cooled to 0 °C and then TMSCl (5.32 g, 6.22 mL, 49.0 mmol, 2.50 equiv.) was added dropwise over the course of five minutes resulting in the formation of copious amounts of white precipitate. The reaction mixture was then allowed to stir at room temperature for 30 minutes and then diluted with Et_2O (5 mL). The solution was filtered by cannula and the precipitate was rinsed with Et_2O (2 x 5 mL). The volatiles were removed *in vacuo* and the crude residue was vacuum distilled to give **5** (0.005 mbar, 80-90 °C) as a colourless, foul-smelling oil.
Yield: 68%, 4.03 g, 13.3 mmol (lit. 90%, 89.7 g);
^{1}H NMR (300 MHz, $CDCl_3$, δ_H): 0.08 (s, 9H), 7.05-7.18 (m, 6H), 7.26-7.33 (m, 4H);
^{13}C{^{1}H} NMR (75.3 MHz, $CDCl_3$, δ_C): -0.60, 127.4, 128.6, 134.4, 137.5;

Synthesis of Ph_2AsH (**12**):
This synthetic approach was closely adapted from a literature procedure.[9] To a THF solution (15 mL) of $AsPh_3$ (6.55 g, 21.4 mmol, 1 equiv.) cooled to 0 °C was added solid lithium sand (324 mg, 46.6 mmol, 2.15 equiv.) slowly over the course of five minutes, resulting in a deep red solution. The reaction mixture was allowed to stir for three hours after warming to room temperature. The solution was then cooled to 0 °C and then degassed H_2O (963 mg, 0.963 mL, 53.5 mmol, 2.50 equiv.) was added

dropwise over the course of five minutes resulting in the formation of a generous amount of white precipitate. The solution was filtered and the precipitate was generously rinsed with Et_2O and then filtered. The combined organic phases were dried with a small amount of Na_2SO_4, filtered, and the volatiles were removed *in vacuo*. The colourless oil obtained was typically pure enough for subsequent chemistry, however vacuum distillation of the product can further purify Ph_2AsH if necessary.

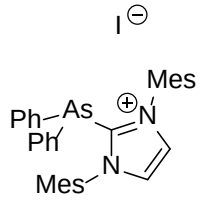
Yield: 81%, 3.98 g, 17.3 mmol (lit. 70%, 3.2 g, Ph_2AsD with distillation);

^{1}H NMR (300 MHz, $CDCl_3$, δ_H): 4.85 (s, 1H), 7.16-7.26 (m, 6H), 7.38-7.45 (m, 4H);

^{13}C{^{1}H} NMR (75.3 MHz, $CDCl_3$, δ_C): 128.3, 128.8, 134.7, 136.6;

Synthesis of Cationic Arsine Ligands:

Synthesis of **2**:



To a stirred toluene solution (3 mL) of Ph_2AsI (268 mg, 0.753 mmol) was added a toluene solution (3 mL) of IMes (229 mg, 0.753 mmol) by cannula transfer, which resulted in the immediate formation of a colourless precipitate. The flask was sealed and sonicated until the precipitate was a free flowing white powder. The filtrate was removed by cannula filtration, and the solids were washed with toluene (3 x 3 mL) and the residual volatiles were removed *in vacuo* to give a colourless air and moisture sensitive solid.

Yield: 94%, 468 mg, 0.708 mmol;

^{1}H NMR (400 MHz, CD_3CN, δ_H): 1.99 (s, 12H), 2.20 (s, 6H), 6.74 (s, 4H), 7.14-7.20 (m, 4H), 7.26-7.30 (m, 4H), 7.32-7.35 (m, 2H), 7.76 (s, 2H);

^{13}C{^{1}H} NMR (100.5 MHz, CD_3CN, δ_C): 18.3, 20.9, 128.3, 129.8, 130.5, 131.1, 131.8, 131.9, 134.9, 135.1, 142.2, 149.3;

FT-IR (ν, cm^{-1}): 456, 479, 667, 691, 705, 724, 736, 746, 783, 849, 856, 999, 1033, 1074, 1231, 1313, 1378, 1433, 1480, 1537, 1606, 2935, 3007;

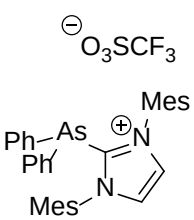
ESI-MS (m/z): 533.2 $[M - I^-]^+$, 126.9 $[I^-]^-$;

HRMS (m/z): calculated for $C_{33}H_{34}As_1N_2$ $[M - I^-]^+$: 533.193225; found: 533.192600 (1.17 ppm).

General Procedure for Anion Exchange of **2**:

To a THF solution (5 mL) of **2** was added solid $AgBF_4$ or AgOTf, which resulted in the immediate formation of a yellow precipitate. The reaction mixture was stirred for 1 hour, after which the solids were allowed to settle. The filtrate was removed by cannula filtration and the precipitate was washed with THF (1 x 2 mL). The volatiles were removed from the combined filtrates *in vacuo* to furnish a colourless solid. No evidence of I^- anions were observed in the ESI(-). These compounds are significantly more stable in the solid-state and in solution than the analogous compound containing I^- as anion (**2**).

Compound **3**.



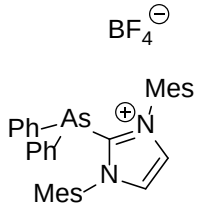
Reagents: **2** (130 mg, 0.197 mmol), AgOTf (55.6 mg, 0.217 mmol, 1.1 equiv.)

Yield: 94%, 126 mg, 0.185 mmol;

^{1}H NMR (400 MHz, CD_3CN, δ_H): 1.95 (s, 12H), 2.20 (s, 6H), 6.74 (s, 4H), 7.15-7.21 (m, 4H), 7.25-7.29 (m, 4H), 7.31-7.36 (m, 2H), 7.70

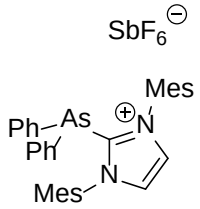
(s, 2H);
$^{13}C\{^{1}H\}$ NMR (100.5 MHz, CD_3CN, δ_C): 18.3, 20.9, 128.3, 129.9, 130.5, 131.2, 131.9, 132.0, 135.0, 135.2, 142.3, 149.5;
$^{19}F\{^{1}H\}$ NMR (282.4 MHz, CD_3CN, δ_F): -78.6;
FT-IR (ν, cm^{-1}): 455, 472, 516, 571, 635, 695, 742, 853, 930, 999, 1029, 1074, 1145, 1222, 1261, 1382, 1438, 1481, 1553, 1608, 2921;
ESI-MS (m/z): 533.2 $[M - OTf^-]^+$, 149.0 $[OTf^-]^-$;
HRMS (m/z): calculated for $C_{33}H_{34}As_1N_2$ $[M - OTf^-]^+$: 533.193225; found: 533.194140 (-1.72 ppm).

Compound **$3BF_4$**.



Reagents: **2** (488 mg, 0.739 mmol), $AgBF_4$ (158 mg, 0.813 mmol, 1.1 equiv.);
Yield: 98%, 449 mg, 0.724 mmol;
^{1}H NMR (400 MHz, $CDCl_3$, δ_H): 1.96 (s, 12H), 2.21 (s, 6H), 6.68 (s, 4H), 7.13-7.20 (m, 8H), 7.28-7.33 (m, 2H), 7.72 (s, 2H);
$^{13}C\{^{1}H\}$ NMR (100.5 MHz, $CDCl_3$, δ_C): 18.1, 21.1, 128.3, 129.1, 129.9, 130.5, 130.7, 130.9, 134.0, 134.1, 141.5, 147.3;
$^{11}B\{^{1}H\}$ NMR (96.3 MHz, CD_3CN, δ_B): -1.18;
$^{19}F\{^{1}H\}$ NMR (282.4 MHz, CD_3CN, δ_F): -151.81 ($^{10}BF_4$), -151.87 ($^{11}BF_4$);
FT-IR (ν, cm^{-1}): 454, 468, 520, 564, 574, 693, 743, 767, 802, 850, 928, 996, 1031, 1044, 1230, 1261, 1362, 1439, 1479, 1556, 1606, 2963, 3124;
ESI-MS (m/z): 533.2 $[M - BF_4^-]^+$, 87.0 $[BF_4^-]^-$;
HRMS (m/z): calculated for $C_{33}H_{34}As_1N_2$ $[M - BF_4^-]^+$: 533.193225; found: 533.193450 (-0.42 ppm).

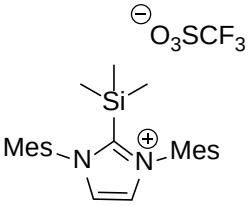
Compound **$3SbF_6$**.



Reagents: **$3BF_4$** (100 mg, 0.161 mmol), $NaSbF_6$ (83.4 mg, 0.322 mmol, 2.0 equiv.);
Yield: 85%, 106 mg, 0.137 mmol;
^{1}H NMR (400 MHz, $CDCl_3$, δ_H): 1.97 (s, 12H), 2.22 (s, 6H), 6.71 (s, 4H), 7.14-7.20 (m, 8H), 7.28-7.33 (m, 2H), 7.57 (s, 2H);
$^{13}C\{^{1}H\}$ NMR (100.5 MHz, $CDCl_3$, δ_C): 18.0, 21.1, 127.8, 129.2, 129.2, 130.0, 130.6, 130.6, 130.9, 134.1, 134.2, 141.7, 147.8;
$^{19}F\{^{1}H\}$ NMR (282.4 MHz, CD_3CN, δ_F): -106.9, -111.0, -113.7, -114.7, -118.4, -120.6, -122.1, -125.9, -127.4, -129.6, -133.3, -134.3, -137.0, -141.1;
FT-IR (ν, cm^{-1}): 455, 471, 488, 574, 652, 695, 742, 796, 855, 931, 1020, 1075, 1230, 1260, 1382, 1438, 1481, 1608, 2963;

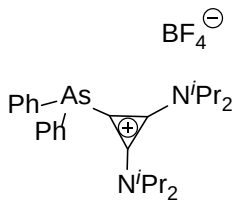
ESI-MS (m/z): 533.2 $[M - SbF_6^-]^+$, 234.9 $[SbF_6^-]^-$;
HRMS (m/z): calculated for $C_{33}H_{34}As_1N_2$ $[M - SbF_6^-]^+$: 533.193225; found: 533.193500 (-0.52 ppm).

Compound **4**.



To a stirred CH_2Cl_2 solution (5 mL) of **2** (138 mg, 0.209 mmol) was added TMSOTf (55.7 mg, 45.4 μL, 0.251 mmol, 1.2 equiv.), which resulted in the immediate formation of a yellow/orange colour. The reaction mixture was allowed to stir for 1 hour, after which the volatiles were removed *in vacuo*. The resulting residue was washed with Et_2O (4 x 4 mL), until the filtrate was no longer yellow. The solids were dried *in vacuo* to give an off-white powder, determined to be **4** by typical characterization methods. The volatiles were removed filtrate *in vacuo* to give a yellow oil which was determined to be **1** by comparison of the NMR spectral data to an authentic sample.
Yield of 1: 95%, 71.0 mg, 0.199 mmol;
Yield of 4: 93%, 102 mg, 0.197 mmol;
Data for **4**:
^{1}H NMR (400 MHz, $CDCl_3$, δ_H): 0.15 (s, 9H), 2.07 (s, 12H), 2.39 (s, 6H), 7.07 (s, 4H), 7.88 (s, 2H);
^{13}C{^{1}H} NMR (100.5 MHz, $CDCl_3$, δ_C): -1.5, 17.6, 21.4, 120.7 (q, $^1J_{F\text{-}C}$ = 319 Hz), 124.9, 128.9, 130.0, 132.0, 134.7, 142.0;
^{19}F{^{1}H} NMR (282.4 MHz, $CDCl_3$, δ_F): -78.4;
FT-IR (ν, cm^{-1}): 516, 572, 636, 715, 753, 775, 845, 933, 1030, 1081, 1146, 1223, 1263, 1384, 1416, 1485, 1556, 1607, 2925;
ESI-MS (m/z): 377.2 $[M - OTf^-]^+$, 149.0 $[OTf^-]^-$;
HRMS (m/z): calculated for $C_{24}H_{33}N_2Si_1$ $[M - OTf^-]^+$: 377.240751; found: 377.240820 (-0.18 ppm).

Synthesis of **6**:



To a THF slurry (20 mL) of 1-chloro-2,3-bis(diisopropylamino) cyclopropenium tetrafluoroborate (2.00 g, 5.58 mmol) was added $Ph_2As(SiMe_3)$ (**1**) (1.69g, 1.30 mL, 5.58 mmol, neat) dropwise by syringe. The flask was sealed under argon and heated at 60 °C for 16 hours. After cooling to room temperature the mixture was filtered and the solvent was removed from the filtrate *in vacuo*. The resulting residue was washed with Et_2O (3 x 8 mL) to give a dark orange oil which was subjected to flash silica gel chromatography (9:1 CH_2Cl_2:Acetone; Rf = 0.27). The main fractions

were combined, the solvent was removed *in vacuo*, and layering a concentrated CH_2Cl_2 solution with MeO^tBu gave analytically pure colourless single crystals of **6**. Compound **6** is stable in the presence of air and moisture indefinitely in the solid-state or in solution.

Yield: 54%, 1.65 g, 5.58 mmol;

^{1}H NMR (400 MHz, $CDCl_3$, δ_H): 1.06 (d, 12H, $^3J_{H\text{-}H}$ = 6.8 Hz), 1.34 (d, 12H, $^3J_{H\text{-}H}$ = 6.8 Hz), 3.46 (sept, 2H, $^3J_{H\text{-}H}$ = 6.8 Hz), 4.08 (sept, 2H, $^3J_{H\text{-}H}$ = 6.8 Hz), 7.40-7.50 (m, 10H);

^{13}C{^{1}H} NMR (100.5 MHz, $CDCl_3$, δ_C): 21.0, 21.4, 52.6, 53.0, 105.8, 129.9, 130.4, 133.7, 134.0, 141.2;

^{11}B{^{1}H} NMR (96.3 MHz, $CDCl_3$, δ_B): -0.98;

^{19}F{^{1}H} NMR (282.4 MHz, $CDCl_3$, δ_F): -153.31 ($^{10}BF_4$), -153.37 ($^{11}BF_4$);

FT-IR (ν, cm^{-1}): 472, 520, 571, 636, 672, 695, 742, 1042, 1095, 1153, 1186, 1357, 1375, 1456, 1544, 1868, 2937, 2986;

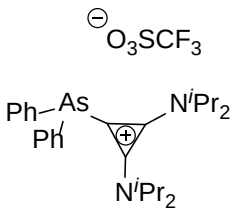
ESI-MS (m/z): 465.2 $[M - BF_4^-]^+$;

HRMS (m/z): calculated for $C_{27}H_{38}As_1N_2$ $[M - BF_4^-]^+$: 465.224525; found: 465.224640 (-0.25 ppm).

General Procedure for Anion Exchange to prepare **7** and **8**:

To a MeCN solution (10 mL) of **6** in a round bottom under ambient conditions was added excess solid KOTf (**7**) or $NaSbF_6$ (**8**). The reaction mixture was allowed to stir overnight, after which the solvent was removed *in vacuo*, and then CH_2Cl_2 (5 mL) was added to the crude solids. The solution was filtered and the solids were washed once more with CH_2Cl_2 (3 mL). The solvent from the combined fractions was removed *in vacuo* to give pure white powders with complete BF_4^- removal, confirmed by $^{11}B\{^1H\}$ and $^{19}F\{^1H\}$ NMR spectroscopy, and also mass spectrometry. Like compound **6**, compounds **7** and **8** are air and moisture stable indefinitely in the solid-state and in solution.

Compound **7**:



Reagents: **6** (175 mg, 0.317 mmol), KOTf (238 mg, 1.267 mmol, 4.0 equiv.)

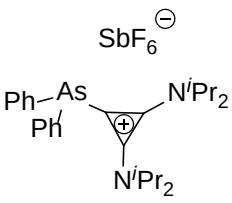
Yield: 98%, 190 mg, 0.311 mmol;

^{1}H NMR (400 MHz, $CDCl_3$, δ_H): 1.09 (d, 12H, $^3J_{H\text{-}H}$ = 6.8 Hz), 1.39 (d, 12H, $^3J_{H\text{-}H}$ = 6.8 Hz), 3.50 (sept, 2H, $^3J_{H\text{-}H}$ = 6.8 Hz), 4.12 (sept, 2H, $^3J_{H\text{-}H}$ = 6.8 Hz), 7.40-7.50 (m, 10H);

^{13}C{^{1}H} NMR (100.5 MHz, $CDCl_3$, δ_C): 21.0, 21.5, 52.8-53.5 (br), 105.9, 120.3 (q, $^1J_{F\text{-}C}$ = 319 Hz), 129.9, 130.5, 133.7, 134.0, 141.3;

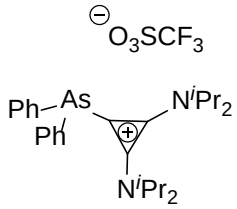
$^{19}F\{^1H\}$ NMR (282.4 MHz, $CDCl_3$, δ_F): -78.1;
FT-IR (ν, cm^{-1}): 480, 515, 570, 634, 667, 695, 734, 1029, 1134, 1184, 1220, 1280, 1351, 1376, 1434, 1458, 1551, 1867, 2981;
ESI-MS (m/z): 465.2 $[M - OTf^-]^+$, 149.0 $[OTf^-]^-$;
HRMS (m/z): calculated for $C_{27}H_{38}As_1N_2$ $[M - OTf^-]^+$: 465.224525; found: 465.224560 (-0.08 ppm).

Compound **8**:



Reagents: **6** (168 mg, 0.304 mmol), $NaSbF_6$ (157 mg, 0.608 mmol, 2 equiv.)
Yield: 88%, 187 mg, 0.268 mmol;
^1H NMR (300 MHz, $CDCl_3$, δ_H): 1.07 (d, 12H, $^3J_{H-H}$ = 6.8 Hz), 1.39 (d, 12H, $^3J_{H-H}$ = 6.8 Hz), 3.47 (sept, 2H, $^3J_{H-H}$ = 6.8 Hz), 4.06 (sept, 2H, $^3J_{H-H}$ = 6.8 Hz), 7.40-7.50 (m, 10H);
$^{13}C\{^1H\}$ NMR (100.5 MHz, $CDCl_3$, δ_C): 21.0, 21.3, 52.9 (br), 106.0, 129.9, 130.4, 133.7, 134.0, 141.3;
$^{19}F\{^1H\}$ NMR (282.4 MHz, $CDCl_3$, δ_F): -106.1, -113.4, -120.3, -127.2, -136.4, -141.4;
FT-IR (ν, cm^{-1}): 482, 573, 650, 695, 735, 747, 854, 899, 1034, 1143, 1155, 1183, 1208, 1352, 1377, 1391, 1434, 1458, 1552, 1869, 2983;
ESI-MS (m/z): 465.2 $[M - SbF_6^-]^+$, 234.9 $[SbF_6^-]^-$;
HRMS (m/z): calculated for $C_{27}H_{38}As_1N_2$ $[M - SbF_6^-]^+$: 465.224525; found: 465.224020 (1.09 ppm).

Direct Synthesis of **7** from $Ph_2As(SiMe_3)$ (**5**):



To a rigorously stirred THF slurry (10 mL) of 1-iodo-2,3-bis(diisopropylamino)cyclopropenium triflate (1.20 g, 2.35 mmol) was added was added $Ph_2As(SiMe_3)$ (**1**) (710 mg, 0.60 mL, 2.35 mmol, neat) dropwise by syringe. The flask was sealed under argon and heated at 60 °C for 16 hours. After cooling to room temperature the mixture was filtered and the solvent was removed from the filtrate *in vacuo*. The resulting residue was washed with Et_2O (5 x 5 mL) giving a light yellow powder that was determined to be pure **7** without the purification procedures necessary for **5** (column chromatography, recrystallization). Single crystals suitable for X-ray analysis were grown from layering a CH_2Cl_2 solution with MeO^tBu. Characterization data was identical to the anion exchange product.
Yield: 85%, 1.23 g, 2.00 mmol

The generated TMSI was found to quantitatively ring open a THF molecule to give $TMSO(CH_2)_4I$ and not polymerize the solvent. For reasons that were not determined, polymerized THF solvent was found to be a problem in some other cases with cationic substituents that were not cyclopropenium based.

NOTE: The analogous reaction with 1-iodo-2,3-bis(diisopropylamino)cyclopropenium salts with different counterions (ie. BF_4^- and SbF_6^-) does not proceed effectively. In the case of the BF_4^- salt a similar quantity of cationic arsine was cleanly isolated, however BF_3 is also produced (presence confirmed by NMR spectroscopy) and a mixture of counteranions (BF_4^-, I^-, I_3^-, confirmed by ESI-MS(-)) were observed. This is likely due to the reaction of the BF_4^- anion with the trimethylsilyl cation generated in the reaction. In the case of the SbF_6^- salt minimal conversion was observed after 2 days, possibly due to the low solubility of the cyclopropenium salt, even in THF at 65 °C. Therefore, to generate the salts with these anions the ion exchange protocol is recommended. Anion exchange of OTf^- (**7**) to SbF_6^- (**8**) was also possible, however in order to obtain to full conversion the following procedure is necessary: To a saturated aqueous $NaSbF_6$ solution was added a DCM solution of the arsine. The organic phase was quickly extracted (2 minutes), dried with $NaSO_4$, and the volatiles were removed *in vacuo* to give compound **8** (ca. 90% yield, 100% conversion). The approach outlined previously (exchanging BF_4^- to other anions using MeCN as the solvent) results in approximately 80-90% SbF_6^- incorporation to the arsine (determined by $^{19}F\{^1H\}$ NMR spectroscopy).

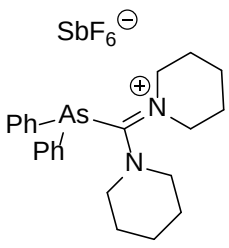
Synthesis of 1-iodo-2,3-bis(diisopropylamino)cyclopropenium triflate:

To a DCM (30 mL) solution of tetrachlorocyclopropene (5.8 ml, 50.5 mmol) at -78 °C was added di-iso-propylamine (28.3 ml, 201 mmol) within 1 hour *via* a dropping funnel. The reaction mixture was stirred overnight and the temperature was allowed to slowly reach room temperature. The reaction mixture was diluted with DCM (20 mL), and KCF_3SO_3 (12.4 g, 65.7 mmol in 50 mL water) was added. After stirring for 20 minutes the organic phase was washed with water (4 x 40 mL), dried over Na_2SO_4, concentrated and dried *in vacuo*. The crude solids were washed with THF (3 x 10 mL) and dried *in vacuo* to give 1-chloro-2,3-bis(diisopropylamino)cyclopropenium triflate.
Yield: 77%, 16.4 g, 38.9 mmol;
^{1}H NMR (400 MHz, CD_3CN, δ_H): 1.32 (overlapping doublets, 24H, $^3J_{H\text{-}H}$ = 6.8 Hz), 3.93 (sept, 2H, $^3J_{H\text{-}H}$ = 6.8 Hz), 3.99 (sept, 2H, $^3J_{H\text{-}H}$ = 6.8 Hz);
$^{13}C\{^1H\}$ NMR (100.5 MHz, CD_3CN, δ_C): 20.5, 23.6, 48.9, 58.8, 93.7, 122.1 (q, $^1J_{F\text{-}C}$ = 319 Hz), 133.4;
$^{19}F\{^1H\}$ NMR (282.4 MHz, CD_3CN, δ_F): -79.2;

FT-IR (ν, cm^{-1}): 516, 541, 570, 634, 749, 893, 1029, 1061, 1134, 1181, 1220, 1266, 1349, 1375, 1422, 1470, 1578, 1920, 2981;
ESI-MS (m/z): 271.2 $[M - OTf^-]^+$, 691.3 $[2M - OTf^-]^+$, 149.0 $[OTf^-]^-$;
HRMS (m/z): calculated for $[M - OTf^-]^+$: 271.193551; found: 271.193470 (0.30 ppm).

The chlorine – iodine exchange reaction was performed once and not optimized.[3] To a mixture of solid 1-chloro-2,3-bis(diisopropylamino)cyclopropenium triflate (6.84 g, 16.3 mmol) and KI (8.92 g, 53.7 mmol) was added standard grade acetone (100 ml) under ambient conditions. The reaction mixture was stirred for 3 hours and a white precipitate was formed. The solvent was removed *in vacuo* and the residue was dissolved in DCM (30 mL) and water. The organic phase was then washed with a saturated aqueous solution of KOTf (3 × 25 mL). Once dried over Na_2SO_4, the organic phase was concentrated and dried *in vacuo*. The ^{1}H NMR spectrum revealed incomplete conversion. The solids were again stirred for 3 hours with an excess of KI (~ 9 g, 54 mmol), and the work up was analogous to the first reaction. The dried precipitate was further washed with THF and the bright yellow powder was dried *in vacuo* to give 1-iodo-2,3-bis(diisopropylamino)cyclopropenium triflate. While this compound is still reasonably soluble in MeCN it is considerably less soluble than the analogous chlorocyclopropenium triflate compound described above.
Yield: 89%, 7.41 g, 14.5 mmol;
^{1}H NMR (300 MHz, CD_3CN, δ_H): 1.29 (d, 12H, $^3J_{H\text{-}H}$ = 6.8 Hz), 1.41 (d, 12H, $^3J_{H\text{-}H}$ = 6.9 Hz), 3.97 (sept, 2H, $^3J_{H\text{-}H}$ = 6.8 Hz), 4.13 (sept, 2H, $^3J_{H\text{-}H}$ = 6.9 Hz);
^{13}C{^{1}H} NMR (100.5 MHz, CD_3CN, δ_C): 20.6, 22.7, 49.3, 54.9, 58.7, 141.3, triflate signal not observed due to solubility of sample at room temperature in CD_3CN;
^{19}F{^{1}H} NMR (282.4 MHz, CD_3CN, δ_F): -79.3;
FT-IR (ν, cm^{-1}): 550, 635, 890, 1030, 1137, 1152, 1208, 1270, 1314, 1346, 1373, 1453, 1553, 1870, 2972;
ESI-MS (m/z): 363.1 $[M - OTf^-]^+$, 126.9 $[I^-]^-$, 149.0 $[OTf^-]^-$;
HRMS (m/z): calculated for $[M - OTf^-]^+$: 363.129170; found: 363.128720 (1.24 ppm).

Synthesis of **9**:



To a THF solution (20 mL) of di(piperidin)formamidinium hexafluoroantimonate (448 mg, 0.992 mmol) was added $Ph_2As(SiMe_3)$ (**5**) (300 mg, 0.231 mL, 0.992 mmol, neat) dropwise by syringe. The flask the sealed under argon and heated at 60 °C for 20 hours. After cooling to room temperature the filtrate was

separated from the precipitate by cannula filtration and after rinsing the precipitate with THF (1 x 3 mL) the volatiles from the combined THF fractions were removed *in vacuo*. The resulting residue was washed and sonicated with Et_2O (4 x 4 mL) before filtering through a short silica plug (2:3 ethylacetate:DCM) and removing the remaining volatiles *in vacuo* to give an off-white solid.

Yield: 62%, 396 mg, 0.614 mmol;

^{1}H NMR (400 MHz, CD_2Cl_2, δ_H): 1.32-1.44 (m, 8H), 1.52-1.63 (m, 4H), 3.69 (t, 8H, $^3J_{H-H}$ = 5.5 Hz), 7.40-7.46 (m, 4H), 7.50-7-57 (m, 6H);

^{13}C{^{1}H} NMR (100.5 MHz, CD_2Cl_2, δ_C): 23.3, 26.7, 55.5, 130.8, 131.1, 133.6, 133.7, 182.9;

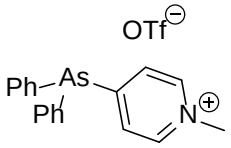
^{19}F{^{1}H} NMR (282.4 MHz, CD_2Cl_2, δ_F): -106.6, -111.5, -120.4, -127.9, -136.4, -141.3

FT-IR (ν, cm^{-1}): 472, 653, 695, 741, 780, 854, 926, 1008, 1091, 1132, 1162, 1251, 1271, 1365, 1436, 1547, 1679, 2860, 2941;

ESI-MS (m/z): 409.2 $[M - SbF_6^-]^+$, 234.9 $[SbF_6^-]^-$;

HRMS (m/z): calculated for $C_{23}H_{30}As_1N_2$ $[M - SbF_6^-]^+$: 409.161925; found: 409.161500 (1.04 ppm).

Synthesis of **10**:



To a $C_2H_4Cl_2$ (1,2-DCE) slurry (8 mL) of 1-methyl-4-iodo-pyridinium trifluoromethanesulfonate (500 mg, 0.677 mmol) was added $Ph_2As(SiMe_3)$ (**5**) (409 mg, 0.340 mL, 0.677 mmol, neat) and the reaction mixture was sealed and stirred for 16 hours at 70 °C. At this time the precipitate was allowed to settle and the dark orange filtrate was isolated by cannula filtration. The volatiles were removed *in vacuo* and the resulting residue was washed and sonicated with Et_2O (4 x 4 mL) to give a viscous orange oil that solidified to a light orange powder upon removing the residual solvents *in vacuo*. While the compound is slightly hydroscopic over time, it is able be weighed and handled under ambient conditions and analysis was performed using solvents that had not been succumbed to special drying procedures.

Yield: 85%, 540 mg, 1.15 mmol;

^{1}H NMR (400 MHz, $CDCl_3$, δ_H): 4.41 (s, 3H), 7.34-7.46 (m, 10H), 7.71 (d, 2H, $^3J_{H-H}$ = 6.4 Hz), 8.63 (d, 2H, $^3J_{H-H}$ = 6.4 Hz);

^{13}C{^{1}H} NMR (100.5 MHz, $CDCl_3$, δ_C): 48.4, 120.2 (q, $^1J_{F-C}$ = 320 Hz), 129.9, 130.4, 131.9, 134.2, 135.5, 143.7, 167.4;

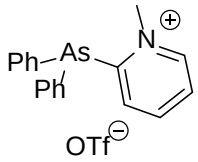
^{19}F{^{1}H} NMR (282.4 MHz, $CDCl_3$, δ_F): -79.1;

FT-IR (ν, cm^{-1}): 460, 473, 503, 517, 572, 599, 639, 666, 695, 712, 737, 755, 809, 833, 999, 1032, 1077, 1152, 1190, 1224, 1261, 1327, 1432, 1455, 1503, 1628, 3042, 3114;

ESI-MS (m/z): 322.1 $[M - OTf^-]^+$, 793.1 $[2M - OTf^-]^+$, 149 $[OTf^-]^-$;

HRMS (m/z): calculated for $C_{18}H_{17}As_1N_1$ [M – OTF^-]$^+$: 322.057126; found: 322.057170 (-0.14 ppm).

Synthesis of **11**:



To a colourless DCE (8 mL) solution of 1-methyl-2-iodo-pyridinium trifluoromethanesulfonate (500 mg, 1.355 mmol) was added $Ph_2As(SiMe_3)$ (**5**) (368 mg, 0.307 mL, 1.22 mmol, 0.9 equiv., neat) dropwise by syringe and the reaction mixture was heated at 70 °C for 16 hours. The dark orange solution was cooled, filtered by cannula filtration, and the volatiles were removed from the filtrate *in vacuo*. The crude residue was washed with Et_2O (4 x 5 mL) and dried *in vacuo*. The solids were determined to have a similar ratio of the product and 1-methyl-2-trimethylsilylpyridinium trifluoromethanesulfonate byproduct (see below for characterization). The product was isolated by flash silica gel column chromatography with the eluent being a 1:9 MeOH:Ethylacetate mixture (Rf = 0.15-0.2). The compound is a white solid which is stable to air and moisture in solution and in the solid state. Single crystals suitable for X-ray analysis were grown from a saturated MeCN:Et_2O vapour diffusion at room temperature.

Yield: 38%, 220 mg, 0.467 mmol (based on $Ph_2As(SiMe_3)$);

^{1}H NMR (400 MHz, $CDCl_3$, δ_H): 4.42 (s, 3H), 7.30-7.35 (m, 4H), 7.42 (dd, 1H, $^3J_{H-H}$ = 7.8 Hz, $^4J_{H-H}$ = 1.6 Hz), 7.43-7.52 (m, 6H), 8.02 (ddd, 1H, $^3J_{H-H}$ = 7.8 Hz, $^3J_{H-H}$ = 6.4 Hz, $^4J_{H-H}$ = 1.6 Hz), 8.20 (dd, 1H, $^3J_{H-H}$ = 7.6 Hz, $^3J_{H-H}$ = 6.4 Hz), 9.25 (dd, 1H, $^3J_{H-H}$ = 7.6 Hz, $^4J_{H-H}$ = 0.8 Hz);

^{13}C{^{1}H} NMR (100.5 MHz, $CDCl_3$, δ_C): 49.0, 120.7 (q, $^1J_{F-C}$ = 320 Hz), 128.1, 130.4, 131.1, 132.9, 133.2, 134.2, 143.6, 149.7, 164.2;

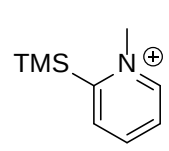
^{19}F{^{1}H} NMR (282.4 MHz, $CDCl_3$, δ_F): -78.3;

FT-IR (ν, cm^{-1}): 435, 470, 485, 516, 572, 635, 698, 714, 747, 778, 998, 1029, 1064, 1149, 1224, 1257, 1440, 1486, 1568, 1608, 3071;

ESI-MS (m/z): 322.1 [M – OTf^-]$^+$, 793.1 [2M – OTf^-]$^+$, 149 [OTf^-]$^-$;

HRMS (m/z): calculated for $C_{18}H_{17}As_1N_1$ [M – OTF^-]$^+$: 322.057126; found: 322.057280 (-0.48 ppm).

Characterization of 1-methyl-2-trimethylsilylpyridinium trifluoromethanesulfonate:

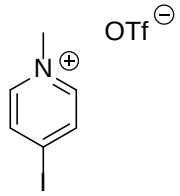


The main byproduct in the synthesis of **11**, 1-methyl-2-trimethylsilylpyridinium trifluoromethanesulfonate, is selectively crystallized from a saturated THF solution of the worked up reaction mixture at 4 °C.

^{1}H NMR (400 MHz, $CDCl_3$, δ_H): 0.58 (s, 9H), 4.52 (s, 3H), 8.00-8.08 (m, overlapping doublets of doublets, 2H), 8.34 (ddd, 1H, $^{3}J_{H\text{-}H}$ = 7.6 Hz, $^{3}J_{H\text{-}H}$ = 6.2 Hz, $^{4}J_{H\text{-}H}$ = 0.8 Hz), 9.14 (dd, 1H, $^{3}J_{H\text{-}H}$ = 7.6 Hz, $^{4}J_{H\text{-}H}$ = 0.8 Hz);
^{13}C{^{1}H} NMR (100.5 MHz, $CDCl_3$, δ_C): 0.8, 49.7, 120.7 (q, $^{1}J_{F\text{-}C}$ = 320 Hz), 128.7, 134.6, 143.0, 149.1,162.7;
^{19}F{^{1}H} NMR (282.4 MHz, $CDCl_3$, δ_F): -78.4;
FT-IR (ν, cm^{-1}): 433, 484, 516, 556, 573, 632, 719, 755, 770, 783, 805, 850, 1028, 1067, 1104, 1143, 1195, 1224, 1255, 1443, 1496, 1608, 3087;
ESI-MS (m/z): 166.1 $[M - OTf^-]^+$, 481.2 $[2M - OTf^-]^+$, 149 $[OTf^-]^-$;
HRMS (m/z): calculated for $C_9H_{16}N_1Si_I$ $[M - OTF^-]^+$: 166.104652; found: 166.104640 (0.07 ppm).

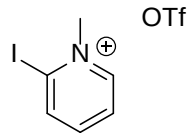
Synthesis of iodopyridinium triflate starting materials:
To a solution of 4-iodopyridine or 2-iodopyridne in toluene (8 mL) was added neat MeOTf (1.5 equiv.), which resulted in the immediate formation of a white precipitate. The mixture was allowed to stir for 30 minutes, after which the precipitate was allowed to settle and the filtrate was removed by cannula filtration. The solids were washed with Et_2O (3 x 5 mL) and the solids were then dried *in vacuo* to give the desired compound as a colourless powder.

1-methyl-4-iodo-pyridinium trifluoromethanesulfonate:



Reagents: 4-iodopyridine (596 mg, 2.91 mmol, 1 equiv.), MeOTf (716 mg, 0.478 mL, 4.36 mmol, 1.5 equiv., neat);
Yield: 96%, 1.04 g, 2.81 mmol;
^{1}H NMR (400 MHz, CD_3CN, δ_H): 4.17 (s, 3H), 8.25 (d, 2H, $^{3}J_{H\text{-}H}$ = 6.4 Hz), 8.40 (d, 2H, $^{3}J_{H\text{-}H}$ = 6.4 Hz);
^{13}C{^{1}H} NMR (100.5 MHz, CD_3CN, δ_C): 49.0, 118.2, 121.7 (q, $^{1}J_{F\text{-}C}$ = 320 Hz), 138.6, 145.5;
^{19}F{^{1}H} NMR (282.4 MHz, CD_3CN, δ_F): -79.1;
FT-IR (ν, cm^{-1}): 479, 516, 572, 633, 701, 756, 804, 829, 1026, 1055, 1081, 1142, 1223, 1252, 1331, 1471, 1495, 1563, 1625, 3046;
ESI-MS (m/z): 220.0 $[M - OTf^-]^+$, 149 $[OTf^-]^-$;
HRMS (m/z): calculated for $C_6H_7I_1N_1$ $[M - OTF^-]^+$: 219.961771; found: 219.961170 (0.32 ppm).

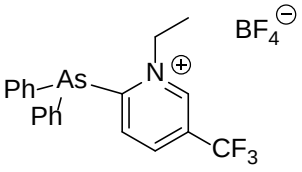
1-methyl-2-iodo-pyridinium trifluoromethanesulfonate:



Reagents: 2-iodopyridine (1.00 g, 4.88 mmol, 1 equiv.), MeOTf (1.20 g, 0.803 mL, 7.32 mmol, 1.5 equiv., neat);

Yield: 94%, 1.69 g, 4.58 mmol;
^{1}H NMR (400 MHz, CD_3CN, δ_H): 4.36 (s, 3H), 7.93 (ddd, 1H, $^{3}J_{H\text{-}H}$ = 7.9 Hz, $^{3}J_{H\text{-}H}$ = 6.2 Hz, $^{4}J_{H\text{-}H}$ = 1.6 Hz), 8.02 (ddd, 1H, $^{3}J_{H\text{-}H}$ = 7.9 Hz, $^{4}J_{H\text{-}H}$ = 1.7 Hz, $^{4}J_{H\text{-}H}$ = 1.6 Hz), 8.54 (dd, 1H, $^{3}J_{H\text{-}H}$ = 8.1 Hz, $^{4}J_{H\text{-}H}$ = 1.6 Hz), 8.91 (dd, 1H, $^{3}J_{H\text{-}H}$ = 6.2 Hz, $^{4}J_{H\text{-}H}$ = 1.7 Hz);
^{13}C{^{1}H} NMR (100.5 MHz, CD_3CN, δ_C): 56.5, 118.4 (overlaps with solvent signal), 121.7 (q, $^{1}J_{F\text{-}C}$ = 320 Hz), 128.3, 142.3, 145.3, 149.2;
^{19}F{^{1}H} NMR (282.4 MHz, CD_3CN, δ_F): -79.2;
FT-IR (ν, cm^{-1}): 431, 478, 515, 572, 634, 703, 756, 777, 974, 1027, 1073, 1085, 1129, 1152, 1179, 1189, 1222, 1251, 1440, 1492, 1502, 1566, 1614, 3081;
ESI-MS (m/z): 220.0 $[M - OTf^-]^+$, 588.9 $[2M - OTf^-]^+$ 149 $[OTf^-]^-$;
HRMS (m/z): calculated for $C_6H_7I_1N_1$ $[M - OTF^-]^+$: 219.961771; found: 219.961970 (-0.90 ppm).

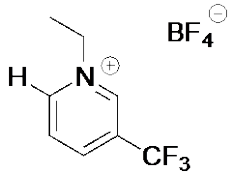
Synthesis of **13**:



To a THF slurry of 1-ethyl-4-trifluoromethyl-2-chloropyridinium tetrafluoroborate (413 mg, 1.39 mmol, 1 equiv.) was added diphenylarsine (**11**) (639 mg, 0.600 mL, 2.78 mmol, 2 equiv., neat) and the resulting mixture was stirred for 72 hours at 70 °C. After cooling to room temperature the filtrate was extracted by cannula filtration and the precipitate was further washed with THF (3 x 3 mL). The precipitate was determined to be mostly starting material, which could be recycled. The solvent was removed from the combined filtrate fractions *in vacuo* and the resulting solid was washed with Et_2O (2 x 3 mL), and toluene (2 x 3 mL). The remaining solid was dried, filtered through a short silica plug (1:1 CH_2Cl_2:Ethylacetate), and the solvent was removed *in vacuo* to give **8** as a colourless powder.
Yield: 19%, 130 mg, 0.264 mmol;
^{1}H NMR (400 MHz, CD_3CN, δ_H): 1.49 (t, 3H, $^{3}J_{H\text{-}H}$ = 7.4 Hz), 4.80 (q, 2H, $^{3}J_{H\text{-}H}$ = 7.4 Hz), 7.41-7.45 (m, 4H), 7.50-7.59 (m, 6H), 7.75 (d, 1H, $^{3}J_{H\text{-}H}$ = 8.4 Hz), 8.46 (dd, 1H, $^{3}J_{H\text{-}H}$ = 8.4 Hz, $^{4}J_{H\text{-}H}$ = 0.6 Hz), 9.21 (s, 1H);
^{13}C{^{1}H} NMR (100.5 MHz, CD_3CN, δ_C): 16.3, 59.2, 122.3 (q, $^{1}J_{F\text{-}C}$ = 272 Hz), 130.8, 130.9 (q, $^{2}J_{F\text{-}C}$ = 35 Hz), 131.8, 134.5, 135.2, 136.3, 141.5 (q, $^{3}J_{F\text{-}C}$ = 3.0 Hz), 146.0, 169.9.
^{11}B{^{1}H} NMR (96.3 MHz, CD_3CN, δ_B): -1.21;
^{19}F{^{1}H} NMR (282.4 MHz, CD_3CN, δ_F): -63.7 (s, 3F), -152.15 ($^{10}BF_4$), -152.21 ($^{11}BF_4$);
FT-IR (ν, cm^{-1}): 477, 520, 690, 740, 859, 997, 1035, 1048, 1108, 1148, 1169, 1188,

1285, 1336, 1404, 1436, 1500, 1577, 1632, 3074;
ESI-MS (m/z): 404.1 $[M - BF_4^-]^+$, 895.1 $[2M - BF_4^-]^+$;
HRMS (m/z): calculated for $C_{20}H_{18}As_1F_3N_1$ $[M - BF_4^-]^+$: 404.060162; found: 404.060080 (0.20 ppm).

Characterization of 1-ethyl-3-trifluoromethylpyridinium tetrafluoroborate:



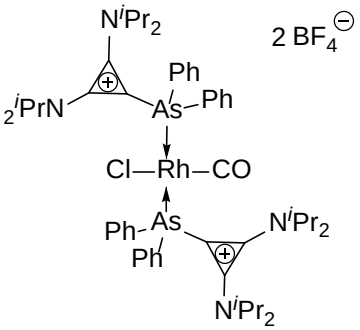
The main byproduct in the synthesis of compound **12**, 1-ethyl-3-trifluoromethylpyridinium tetrafluoroborate, was isolated fairly cleanly by washing the crude solids with DCM and drying the remaining insoluble white powder.

^{1}H NMR (300 MHz, CD_3CN, δ_H): 1.62 (t, 3H, $^3J_{H\text{-}H}$ = 7.5 Hz), 4.67 (q, 2H, $^3J_{H\text{-}H}$ = 7.5 Hz), 8.26 (broad triplet, 1H), 8.79 (d, 1H, $^3J_{H\text{-}H}$ = 8.4 Hz), 8.96 (broad doublet, 1H), 9.21 (s, 1H);
^{11}B{^{1}H} NMR (96.3 MHz, CD_3CN, δ_B): -1.18;
^{19}F{^{1}H} NMR (282.4 MHz, CD_3CN, δ_F): -63.7 (s, 3F), -151.89 ($^{10}BF_4$), -151.95 ($^{11}BF_4$);
FT-IR (ν, cm^{-1}): 435, 522, 586, 676, 687, 742, 810, 824, 854, 945, 1034, 1102, 1145, 1184, 1225, 1334, 1355, 1461, 1492, 1511, 1602, 1655, 3088;
ESI-MS (m/z): 176.1 $[M - BF_4^-]^+$, 439.1 $[2M - BF_4^-]^+$;
HRMS (m/z): calculated for $C_8H_9F_3N_1$ $[M - BF_4^-]^+$: 176.068159; found: 176.068180 (-0.12 ppm).

Synthesis of Rhodium Compounds:

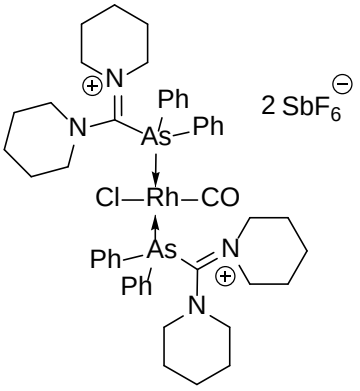
General Procedure for the Preparation of Rhodium Carbonyl Complexes:
To an argon filled Schlenk flask containing solid cationic arsine ligand and $\{Rh(Cl)(CO)_2\}_2$ cooled to -20 °C was added CH_2Cl_2 (2 mL). The reaction mixture was allowed to stir for 30 minutes at this temperature before being allowed to warm up to room temperature for another 30 minutes. The solvent was removed *in vacuo* and the crude solids were washed with Et_2O (3 x 2 mL) to give a yellow solid. Single crystals for X-ray diffraction studies were obtained by layering a CH_2Cl_2 solution with Et_2O.

Synthesis of **14**:



Reagents: **6** (112 mg, 0.203 mmol, 1 equiv.), $\{Rh(Cl)(CO)_2\}_2$ (19.9 mg, 0.051 mmol, 0.25 equiv.);
Yield: 87%, 113 mg, 0.179 mmol;
^{1}H NMR (400 MHz, CD_2Cl_2, δ_H): 0.99 (d, 12H, $^3J_{H\text{-}H}$ = 6.8 Hz), 1.33 (d, 12H, $^3J_{H\text{-}H}$ = 6.8 Hz), 3.51 (sept, 2H, $^3J_{H\text{-}H}$ = 6.8 Hz), 4.10 (sept, 2H, $^3J_{H\text{-}H}$ = 6.8 Hz), 7.60-7.69 (m, 6H), 8.05-8.12 (m, 4H);
^{13}C{^{1}H} NMR (100.5 MHz, CD_2Cl_2, δ_C): 21.3, 21.6, 52.0-54.0 (br), 100.1, 130.7, 131.1, 133.1, 134.8, 141.6, 184.0 (d, $^1J_{Rh\text{-}C}$ = 66.7 Hz);
^{11}B{^{1}H} NMR (96.3 MHz, CD_2Cl_2, δ_B): -1.11;
^{19}F{^{1}H} NMR (282.4 MHz, CD_2Cl_2, δ_F): -152.50 ($^{10}BF_4$), -152.56 ($^{11}BF_4$);
FT-IR (ν, cm^{-1}): 471, 521, 570, 645, 666, 695, 745, 893, 997, 1038, 1056, 1150, 1184, 204, 1355, 1377, 1440, 1454, 1554, 1864, **1968**, 2938, 2976;
ESI-MS (m/z): 1183.3 $[M - BF_4^-]^+$;
HRMS (m/z): calculated for $C_{55}H_{76}As_2BCl_1F_4N_4O_1Rh_1$ $[M - BF_4^-]^+$: 1183.321087; found: 1183.321300 (-0.18 ppm).

Synthesis of **15**:



Reagents: **9** (50 mg, 0.0775 mmol, 1 equiv.), $\{Rh(Cl)(CO)_2\}_2$ (7.61 mg, 0.0194 mmol, 0.25 equiv.);
Yield: 90%, 51.1 mg, 0.0350 mmol;
^{1}H NMR (400 MHz, CD_2Cl_2, δ_H): 1.46-1.52 (br, 8H), 1.56-1.62 (br, 4H), 3.71 (t, 8H, $^3J_{H\text{-}H}$ = 5.6 Hz), 7.62-7-70 (m, 6H), 7.86-7.90 (m, 4H);
^{13}C{^{1}H} NMR (100.5 MHz, CD_2Cl_2, δ_C): 22.9, 26.2, 55.6, 130.9, 131.2, 133.4, 134.4, 174.9, 183.7 (d, $^1J_{Rh\text{-}C}$ = 68.3

Hz);

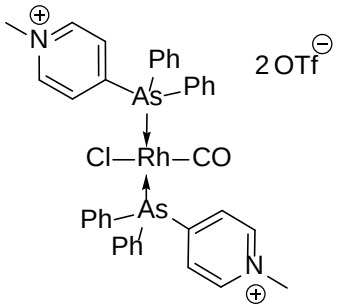
^{19}F{^{1}H} NMR (282.4 MHz, CD_2Cl_2, δ_F): -103.8, -106.5, -113.7, -121.0, -127.7, -137.3, -142.3;

FT-IR (ν, cm^{-1}): 470, 561, 652, 693, 742, 855, 1009, 1070, 1131, 1252, 1364, 1438, 1555, 1679, **1983**, 2944;

ESI-MS (m/z): 492.1 $[M - 2SbF_6^-]^{2+}$, 1219.1 $[M - SbF_6^-]^+$, 234.9 $[SbF_6^-]^-$;

HRMS (m/z): calculated for $C_{47}H_{60}As_2Cl_1F_6N_4O_1Rh_1Sb_1$ $[M - SbF_6^-]^+$: 1219.087137; found: 1219.087770 (-0.52 ppm).

Synthesis of **16**:



Reagents: **10** (55.0 mg, 0.117 mmol, 1 equiv.), $\{Rh(Cl)(CO)_2\}_2$ (11.5 mg, 0.029 mmol, 0.25 equiv.);

Yield: 94%, 60.7 mg, 0.0545 mmol;

^{1}H NMR (400 MHz, CD_2Cl_2, δ_H): 4.35 (s, 3H), 7.50-7.60 (m, 6H), 7.65-7.70 (m, 4H), 8.15 (d, 2H, $^{3}J_{H-H}$ = 6.4 Hz), 8.77 (d, 2H, $^{3}J_{H-H}$ = 6.4 Hz);

^{13}C{^{1}H} NMR (100.5 MHz, CD_2Cl_2, δ_C): 49.1, 120.3 (q, $^{1}J_{F-C}$ = 319 Hz), 130.3, 130.9, 132.2, 133.1, 134.3, 144.7, 157.3, 184.5 (d, $^{1}J_{Rh-C}$ = 66.6 Hz);

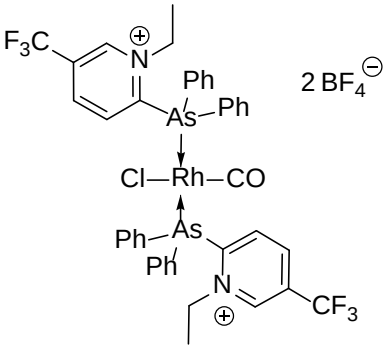
^{19}F{^{1}H} NMR (282.4 MHz, CD_2Cl_2, δ_F): -78.4;

FT-IR (ν, cm^{-1}): 465, 498, 517, 565, 635, 692, 739, 824, 998, 1027, 1077, 1148, 1222, 1253, 1436, 1627, **1979**;

ESI-MS (m/z): 405.0 $[M - 2OTf^-]^{2+}$, 958.9 $[M - OTf^-]^+$, 149 $[OTf^-]^-$;

HRMS (m/z): calculated for $C_{38}H_{34}As_2Cl_1F_3N_1O_4Rh_1S_1$ $[M - OTF^-]^+$: 958.93614; found: 958.937100 (1.00 ppm).

Synthesis of **17**:



Reagents: **13** (34 mg, 0.0692 mmol, 1 equiv.), $\{Rh(Cl)(CO)_2\}_2$ (6.80 mg, 0.0173 mmol, 0.25 equiv.);

Yield: 93%, 37.2 mg, 0.032 mmol;

^{1}H NMR (400 MHz, CD_3CN, δ_H): 1.47 (t, 3H, $^{3}J_{H-H}$ = 7.2 Hz), 4.94 (q, 2H, $^{3}J_{H-H}$ = 7.2 Hz), 7.55-7.65 (m, 10H), 7.78 (d, 1H, $^{3}J_{H-H}$ = 8.4 Hz), 8.51 (dd, 2H, $^{3}J_{H-H}$ = 8.4 Hz, $^{4}J_{H-H}$ = 2.0 Hz), 9.25 (s, 1H);

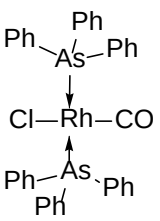
^{13}C{^{1}H} NMR (100.5 MHz, CD_3CN, δ_C): 16.2, 59.5, 122.4 (q, $^{1}J_{F-C}$ = 273 Hz), 131.0, 131.5 (q, $^{2}J_{F-C}$ = 21.6 Hz), 132.3, 133.5, 135.2, 136.2, 141.7 (q, $^{3}J_{F-C}$ = 3.1 Hz), 146.3, 168.2, 183.0 (d, $^{1}J_{Rh-C}$ = 67.1 Hz);

^{11}B{^{1}H} NMR (96.3 MHz, CD_3CN, δ_B): -1.18.

$^{19}F\{^{1}H\}$ NMR (282.4 MHz, CD_3CN, δ_F): -63.7 (s, 3F), -152.00 ($^{10}BF_4$), -152.05 ($^{11}BF_4$).
FT-IR (ν, cm^{-1}): 475, 521, 560, 691, 744, 861, 916, 998, 1034, 1048, 1110, 1152, 1191, 1284, 1355, 1403, 1439, 1496, 1581, 1629, **1999**, 3069;
ESI-MS (m/z): unfortunately, no signal attributable to the product was observed, only for **13** (404.1 $[M - BF_4^-]^+$)

Synthesis of **18**:
To accurately compare CO stretching frequencies with the cationic ligands the $AsPh_3$ (**18**) rhodium complex was also prepared. The reaction were setup in an analogous manner to the general procedure; the difference was that they were performed at room temperature and washed thoroughly with pentane instead of Et_2O. The products were convincingly characterized to confirm the structure and purity, and these data compare well to the reported values.[10-12] A high quality, low temperature X-ray diffraction study was also performed on a sample of **18** grown from a CH_2Cl_2/hexanes vapour diffusion.[11]

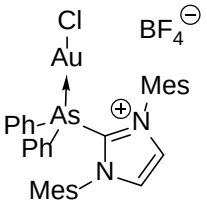
Compound **18**:



Reagents: $AsPh_3$ (78.0 mg, 0.255 mmol, 1 equiv.), $\{Rh(Cl)(CO)_2\}_2$ (25.0 mg, 0.0636 mmol, 0.25 equiv.);
Yield: 96%, 95.2 mg, 0.122 mmol;
^{1}H NMR (300 MHz, $CDCl_3$, δ_H): 7.35-7.44 (m, 6H), 7.65-7.69 (m, 4H);
$^{13}C\{^{1}H\}$ NMR (75.3 MHz, $CDCl_3$, δ_C): 128.8, 130.0, 134.2, 134.8, 183.5-185.5 (br);
FT-IR (ν, cm^{-1}): 472, 571, 693, 727, 999, 1024, 1077, 1158, 1183, 1305, 1434, 1482, 150, **1955**;
ESI-MS (m/z): 800.9 $[M + Na^+]^+$,
HRMS (m/z): calculated for $C_{37}H_{30}As_2Cl_1Na_1O_1Rh_1$ $[M + Na^+]^+$: 800.935693; found: 800.935560 (0.17 ppm).

Synthesis of Metal Complexes with the Cationic Arsine Ligands:

Synthesis of **19**:



To an argon filled Schlenk flask containing **3(BF$_4$)** (45.0 mg, 0.073 mmol) and AuCl(SMe$_2$) (21.4 mg, 0.073 mmol) at room temperature was added CH_2Cl_2 (2 mL). After stirring for 30 minutes *n*-pentane (10 mL) was added, resulting in the formation of a white precipitate. After decanting the filtrate, the solids were washed with pentane (2 x 2 mL) and toluene (2 x 1 mL) to give a colourless powder.

Yield: 92%, 56.9 mg, 0.067 mmol;

^{1}H NMR (400 MHz, $CDCl_3$, δ_H): 2.00 (s, 12H), 2.22 (s, 6H), 6.76 (s, 4H), 7.22-7.30 (br t, 4 H, $^3J_{H-H}$ = 7.6 Hz), 7.39-7.43 (br, 6H), 7.77 (brs, 2H);

^{13}C{^{1}H} NMR (75.3 MHz, $CDCl_3$, δ_C): 18.1, 21.1, 128.5, 129.2, 130.0, 130.6, 130.8, 131.0, 134.0, 134.2, 141.5, 147.4 (br);

^{11}B{^{1}H} NMR (96.3 MHz, CD_3CN, δ_B): -1.18;

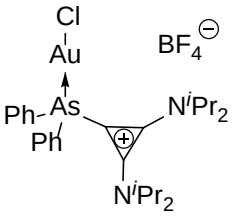
^{19}F{^{1}H} NMR (282.4 MHz, CD_3CN, δ_F): -151.92 ($^{10}BF_4$), -151.98 ($^{11}BF_4$);

FT-IR (ν, cm^{-1}): 455, 473, 485, 522, 563, 574, 696, 743, 752, 776, 789, 848, 928, 997, 1031, 1048, 1230, 1383, 1439, 1478, 1606;

ESI-MS (m/z): 765.1 $[M - BF_4^-]^+$, 87.0 $[BF_4^-]^-$;

HRMS (m/z): calculated for $C_{33}H_{34}As_1Au_1Cl_1N_2$ $[M - BF_4^-]^+$: 765.128631; found: 765.128390 (0.31ppm).

Synthesis of **20**:



A CH_2Cl_2 solution (1 mL) of AuCl(SMe$_2$) (43.7 mg, 0.148 mmol) was added to a stirred CH_2Cl_2 solution (1 mL) of **6** (82.0 mg, 0.148 mmol) at -20 °C. The mixture was allowed to warm up to room temperature over the course of an hour. The product was precipitated from the reaction mixture by adding n-pentane (4 mL). The crude solids were washed with n-pentane (3 x 2 mL) to give a beige powder. This compound is stable under ambient conditions in the solid-state for over a year.

Yield: 89%, 104 mg, 0.133 mmol;

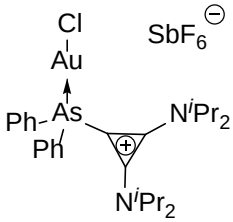
^{1}H NMR (300 MHz, CD_2Cl_2, δ_H): 1.06 (d, 12H, $^3J_{H-H}$ = 6.9 Hz), 1.39 (d, 12H, $^3J_{H-H}$ = 6.9 Hz), 3.49 (sept, 2H, $^3J_{H-H}$ = 6.9 Hz), 4.13 (sept, 2H, $^3J_{H-H}$ = 6.9 Hz), 7.64-7.68 (m, 6H), 7.89-7.93 (m, 4H);

^{13}C{^{1}H} NMR (75.3 MHz, CD_2Cl_2, δ_C): 21.68, 21.70, 53.0-54.0 (br; overlapping with solvent signal), 97.0, 128.6, 131.2, 133.8, 134.5, 140.7;

^{11}B{^{1}H} NMR (96.3 MHz, CD_2Cl_2, δ_B): -1.10;

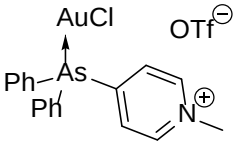
^{19}F{^{1}H} NMR (282.4 MHz, CD_2Cl_2, δ_F): -151.56 ($^{10}BF_4$), -151.61 ($^{11}BF_4$);
FT-IR (ν, cm^{-1}): 458, 469, 521, 573, 643, 691, 741, 895, 997, 1044, 1092, 1145, 1185, 1204, 1359, 1377, 1440, 1568, 1868, 2979;
ESI-MS (m/z): 697.1 $[M - BF_4^-]^+$;
HRMS (m/z): calculated for $C_{27}H_{38}As_1Au_1Cl_1N_2$ $[M - BF_4^-]^+$: 697.159931; found: 697.160430 (-0.72 ppm).

Synthesis of **21**:



Prepared following the procedure already described for **20**. Reagents: **8** (80.0 mg, 0.114 mmol), $AuCl(SMe_2)$ (33.6 mg, 0.114 mmol);
Yield: 96%, 102.3 mg, 0.1090 mmol;
^{1}H NMR (300 MHz, CD_2Cl_2, δ_H): 1.07 (d, 12H, $^{3}J_{H-H}$ = 6.9 Hz), 1.37 (d, 12H, $^{3}J_{H-H}$ = 6.9 Hz), 3.49 (sept, 2H, $^{3}J_{H-H}$ = 6.9 Hz), 4.08 (sept, 2H, $^{3}J_{H-H}$ = 6.9 Hz), 7.53-7.61 (m, 10H);
^{13}C{^{1}H} NMR (100.1 MHz, CD_2Cl_2, δ_C): 21.3, 21.7, 52.0-54.0 (br; overlapping with solvent signal), 97.5, 123.3, 130.7, 132.0, 134.1, 141.1;
^{19}F{^{1}H} NMR (282.4 MHz, CD_2Cl_2, δ_F): -106.4, -110.9, -113.4, -120.6, -127.6, -134.3, -136.9, -141.4;
FT-IR (ν, cm^{-1}): 482, 573, 651, 695, 736, 746, 996, 1033, 1080, 1143, 1183, 1264, 1352, 1376, 1435, 1458, 1552, 1868, 2982;
ESI-MS (m/z): 697.2 $[M - SbF_6^-]^+$, 234.9 $[SbF_6^-]^-$;
HRMS (m/z): calculated for $C_{27}H_{38}As_1Au_1Cl_1N_2$ $[M - SbF_6^-]^+$: 697.160481; found: 697.159680(1.15 ppm).

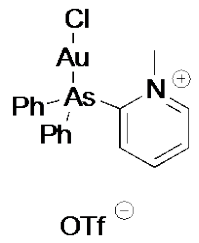
Synthesis of **22**:



To an argon filled Schlenk flask containing **10** (55.0 mg, 0.117 mmol) and $AuCl(SMe_2)$ (34.4 mg, 0.117 mmol) at -20 °C was added CH_2Cl_2 (3 mL). The reaction mixture was allowed to stir for 30 minutes at this temperature before warming to room temperature and stirring for an additional 30 minutes. The solvent was removed *in vacuo* and the crude solids were washed with Et_2O (4 x 3 mL), followed by the thorough drying of solids to give **22** as a light yellow solid.
Yield: 92%, 75.6 mg, 0.107 mmol;
^{1}H NMR (400 MHz, $CDCl_3$, δ_H): 4.46 (s, 3H), 7.50-7.62 (m, 10H), 7.89 (d, 2H, $^{3}J_{H-H}$ = 6.4 Hz), 8.85 (d, 2H, $^{3}J_{H-H}$ = 6.4 Hz);
^{13}C{^{1}H} NMR (75.3 MHz, $CDCl_3$, δ_C): 49.3, 120.3 (q, $^{1}J_{F-C}$ = 319 Hz), 128.3, 130.7, 131.8, 133.0, 133.8, 145.5, 155.0;

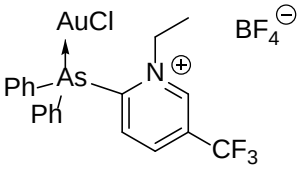
$^{19}F\{^1H\}$ NMR (282.4 MHz, $CDCl_3$, δ_F): -78.4;
FT-IR (ν, cm^{-1}): 464, 499, 517, 572, 635, 691, 740, 825, 997, 1027, 1080, 1148, 1222, 1253, 1437, 1628;
ESI-MS (m/z): 554.0 $[M - OTf^-]^+$, 149 $[OTf^-]^-$;
HRMS (m/z): calculated for $C_{18}H_{17}As_1Au_1Cl_1N_1$ $[M - OTF^-]^+$: 553.992532; found: 553.993400 (-1.57 ppm).

Synthesis of **23**:



To an argon filled Schlenk flask containing **11** (40.0 mg, 0.0850 mmol) and $AuCl(SMe_2)$ (25.0 mg, 0.0850 mmol) at -20 °C was added CH_2Cl_2 (3 mL). The reaction mixture was allowed to stir for 30 minutes at this temperature before warming to room temperature for 5 minutes. At this time the workup proceeds quickly in order to avoid decomposition of the product. The solvent was reduced by ca. 50% *in vacuo* and Et_2O (5 mL) was added, which resulted in the precipitation of a colourless solid. The precipitate was washed with Et_2O (3 x 2 mL) and dried *in vacuo* to give **23** as a white solid. While the product is stable in the solid-state under an argon atmosphere it begins to deposit elemental gold after being in solution for more than a couple hours.
Yield: 95%, 56.7 mg, 0.808 mmol;
^1H NMR (400 MHz, CD_2Cl_2, δ_H): 4.44 (s, 3H), 7.45-7.64 (m, 11H), 8.05 (ddd, 1H, $^3J_{H-H}$ = 8.0 Hz, $^3J_{H-H}$ = 6.4 Hz, $^4J_{H-H}$ = 0.8 Hz), 8.27 (ddd, 1H, $^3J_{H-H}$ = 8.0 Hz, $^3J_{H-H}$ = 6.4 Hz, $^4J_{H-H}$ = 1.6 Hz), 9.16 (dd, 1H, $^3J_{H-H}$ = 6.4 Hz, $^4J_{H-H}$ = 1.6 Hz);
$^{13}C\{^1H\}$ NMR (100.5 MHz, CD_2Cl_2, δ_C): 49.5, 121.1 (q, $^1J_{F-C}$ = 320 Hz), 129.0, 130.9, 131.1, 132.2, 134.0, 134.4, 144.6, 150.3, 160.8;
$^{19}F\{^1H\}$ NMR (282.4 MHz, CD_2Cl_2, δ_F): -78.5;
FT-IR (ν, cm^{-1}): 435, 469, 516, 572, 636, 696, 747, 793, 864, 1026, 1075, 1149, 1224, 1258, 1412, 1438, 1485, 1609, 2963;
ESI-MS (m/z): 544.0 $[M - OTf^-]^+$, 1256.9 $[2M - OTf^-]^+$, 149 $[OTf^-]^-$, 851.9 $[M + OTf^-]^-$;
HRMS (m/z): calculated for $C_{18}H_{17}As_1Au_1Cl_1N_1$ $[M - OTF^-]^+$: 553.992532; found: 553.993150 (-1.12 ppm).

Synthesis of **24**:



To an argon filled Schlenk flask containing **13** (20.0 mg, 0.0407 mmol) and $AuCl(SMe_2)$ (12.0 mg, 0.0407 mmol) cooled to -20 °C was added CH_2Cl_2 (3 mL). The reaction mixture was allowed to stir for 30 minutes at this temperature

before warming to room temperature and stirring for an additional 30 minutes. The solvent was removed *in vacuo* and the crude solids were washed with Et_2O (4 x 3 mL), followed by the thorough drying of solids to give **24** as a colourless solid.

Yield: 96%, 28.3 mg, 0.039 mmol;

^{1}H NMR (400 MHz, CD_3CN, δ_H): 1.49 (t, 3H, $^{3}J_{H\text{-}H}$ = 7.2 Hz), 4.80 (q, 2H, $^{3}J_{H\text{-}H}$ = 7.2 Hz), 7.50-7.65 (m, 10H), 7.78 (d, 1H, $^{3}J_{H\text{-}H}$ = 8.4 Hz), 8.52 (dd, 2H, $^{3}J_{H\text{-}H}$ = 8.4 Hz, $^{4}J_{H\text{-}H}$ = 2.0 Hz), 9.25 (s, 1H);

^{13}C{^{1}H} NMR (100.5 MHz, CD_3CN, δ_C): 16.3, 59.3, 122.3 (q, $^{1}J_{F\text{-}C}$ = 274 Hz), 131.1, 131.5 (q, $^{2}J_{F\text{-}C}$ = 21.6 Hz), 132.6, 135.1, 136.4, 142.1 (q, $^{3}J_{F\text{-}C}$ = 3.8 Hz), 146.6, 166.3;

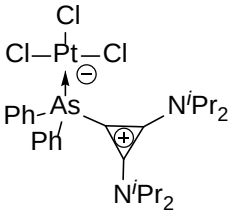
^{11}B{^{1}H} NMR (96.3 MHz, CD_3CN, δ_B): -0.02;

^{19}F{^{1}H} NMR (282.4 MHz, CD_3CN, δ_F): -63.7 (s, 3F), -152.14 ($^{10}BF_4$), -152.20 ($^{11}BF_4$);

FT-IR (ν, cm^{-1}): 467, 478, 521, 693, 740, 858, 997, 1036, 1050, 1115, 1148, 1170, 1225, 1286, 1341, 1405, 1437, 1482, 1501, 1577, 1634, 3073;

ESI-MS (m/z): unfortunately, no signal attributable to the product was observed, only for **12** (404.1 $[M - BF_4^-]^+$).

Synthesis of **25**:



To an argon filled Schlenk flask containing **6** (65.0 mg, 0.118 mmol) and finely ground K_2PtCl_4 (49.0 mg, 0.118 mmol) was added MeCN (4 mL). After the resulting mixture was stirred vigorously for 20 hours the solvent was removed *in vacuo*, and then CH_2Cl_2 (5 mL) was added. The orange solution was filtered and the solvent was removed *in vacuo* to give an orange solid. This compound is stable under ambient conditions in the solid-state for over a year.

Yield: 95%, 104 mg, 0.112 mmol;

^{1}H NMR (400 MHz, CD_3CN, δ_H): 0.88 (d, 12H, $^{3}J_{H\text{-}H}$ = 6.8 Hz), 1.27 (d, 12H, $^{3}J_{H\text{-}H}$ = 6.8 Hz), 3.57 (sept, 2H, $^{3}J_{H\text{-}H}$ = 6.8 Hz), 4.07 (sept, 2H, $^{3}J_{H\text{-}H}$ = 6.8 Hz), 7.55-7.65 (m, 6H), 8.16-8.23 (m, 4H);

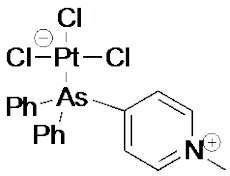
^{13}C{^{1}H} NMR (100.5 MHz, CD_3CN, δ_C): 20.6, 21.5, 52.8, 54.2, 98.9, 129.3, 130.4, 133.1, 135.5, 141.7;

FT-IR (ν, cm^{-1}): 470, 569, 646, 660, 691, 736, 748, 891, 1029, 1078, 1146, 1183, 1352, 1374, 1438, 1450, 1482, 1551, 1864, 2933, 2977;

ESI-MS (m/z): 772 $[M - Cl^- + MeCN]^+$, 789.2 $[M + Na^+]^+$;

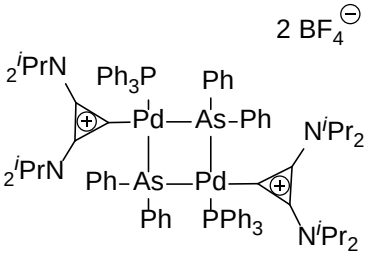
HRMS (m/z): calculated for $C_{27}H_{38}As_1Cl_3N_2Na_1Pt_1$ $[M + Na^+]^+$: 788.085666; found: 788.086000 (-0.42 ppm).

Reaction of **10** with K_2PtCl_4:



To an argon filled Schlenk flask containing **10** and K_2PtCl_4 at room temperature was added MeCN (4 mL) and the reaction was allowed to stir for 16 hours. The volatiles were removed from the orange solution *in vacuo* and the crude solids were rinsed with CH_2Cl_2. The filtrate was isolated by cannula filtration and the volatiles were removed *in vacuo* to give a light orange solid. Analysis of the powder by ^{1}H NMR spectroscopy in CD_2Cl_2 revealed 3 products containing the pyridinium arsine ligand. From this saturated solution single crystals suitable for X-ray analysis were formed and were determined to be the intended product, **26**. Despite considerable effort this compound was always obtained in small amounts.

Synthesis of **27**:



To an argon filled Schlenk flask containing **6** (40.0 mg, 0.072 mmol) and $Pd(PPh_3)_4$ (83.7, 0.072 mmol) was added toluene and the resulting reaction mixture was heated near reflux at 100 °C for 16 hours. The resulting dark orange solution and a light orange precipitate was cooled to room temperature and the filtrate was removed and revealed to contain mostly PPh_3 by $^{31}P\{^1H\}$ NMR spectroscopy. The precipitate was washed with toluene (5 x 2 mL) until the filtrate was no longer orange. The solids were dried *in vacuo* to give **27** as a yellow powder, which was recrystallized by layering a CH_2Cl_2 solution with Et_2O to give single crystals suitable for X-ray diffraction studies.

Yield: 53%, 35.6 mg, 0.0191 mmol;

^{1}H NMR (400 MHz, CD_2Cl_2, δ_H): 0.42 (d, 12H, $^3J_{H\text{-}H}$ = 6.6 Hz), 0.79 (d, 12H, $^3J_{H\text{-}H}$ = 6.6 Hz), 1.02 (d, 12H, $^3J_{H\text{-}H}$ = 6.6 Hz), 1.07 (d, 12H, $^3J_{H\text{-}H}$ = 6.9 Hz), 3.25 (sept, 4H, $^3J_{H\text{-}H}$ = 6.6 Hz), 3.66 (sept, 4H, $^3J_{H\text{-}H}$ = 6.9 Hz), 6.80 (t, 12H, $^3J_{H\text{-}H}$ = 7.8 Hz), 7.12 (t, 12H, $^3J_{H\text{-}H}$ = 7.8 Hz), 7.25 (t, 8H, $^3J_{H\text{-}H}$ = 7.5 Hz), 7.28-7-35 (br, 8H), 7.42 (t, 6H, $^3J_{H\text{-}H}$ = 7.5 Hz), 7.49 (t, 4H, $^3J_{H\text{-}H}$ = 7.5 Hz);

^{13}C{^{1}H} NMR (100.5 MHz, CD_2Cl_2, δ_C): 22.1, 22.8, 49.0-51.0 (br), 128.5 (br), 129.0 (d, $J_{P\text{-}C}$ = 20.5 Hz), 129.8, 130.6, 131.7, 133.0, 133.5 (dd, $J_{P\text{-}C}$ = 13.7 Hz, $J_{P\text{-}C}$ = 2.9 Hz), 134.2 (br), 134.5, 146.5;

^{11}B{^{1}H} NMR (96.3 MHz, CD_2Cl_2, δ_B): -1.11;

^{19}F{^{1}H} NMR (282.4 MHz, CD_2Cl_2, δ_F): -153.45 ($^{10}BF_4$), -153.50 ($^{11}BF_4$);

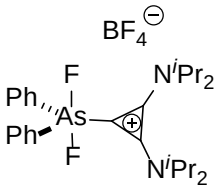
^{31}P{^{1}H} NMR (161.8 MHz, CD_2Cl_2, δ_P): 14.7;

FT-IR (ν, cm^{-1}): 463, 492, 518, 654, 693, 733, 893, 999, 1031, 1048, 1088, 1149, 1183, 1319, 1343, 1371, 1435, 1491, 1844, 2974;

ESI-MS (m/z): 465.2 $[M - BF_4^-]^+$, 941.2 $[M - AsPh_2 - C_3(N^iPr_2)_2 - 2BF_4^-]^+$ (isotope

pattern diagnostic of 2 Pd atoms), other mass signals observed: 573, 678, 832, 1180, 1496;

Synthesis of **28**:



In an argon filled glove box (< 0.5 ppm H_2O and O_2) solid XeF_2 (33.7 mg, 0.199 mmol, 1.1 equiv.) was added to a CH_2Cl_2 solution (1.5 mL) of **6** (100 mg, 0.181 mmol, 1 equiv.) resulting in the evolution of a gas. The reaction mixture was allowed to stir for 1 hour before the solvent was removed *in vacuo*. The crude solids were washed with Et_2O (3 x 1.5 mL) and dried *in vacuo* to give **28** as a colourless powder. Compound **28** is very reasonably sensitive to air and moisture, slowly converting to the oxide, which then decomposes further (see below).

Yield: 98%, 104 mg, 0.175 mmol;

^{1}H NMR (300 MHz, $CDCl_3$, δ_H): 1.16 (d, 12H, $^3J_{H\text{-}H}$ = 6.8 Hz), 1.41 (d, 12H, $^3J_{H\text{-}H}$ = 6.8 Hz), 3.92 (sept, 2H, $^3J_{H\text{-}H}$ = 6.8 Hz), 4.20 (sept, 2H, $^3J_{H\text{-}H}$ = 6.8 Hz), 7.59 (t, 4H, $^3J_{H\text{-}H}$ = 8.1 Hz), 7.67 (m, 2H), 8.21 (m, 4H);

^{13}C{^{1}H} NMR (100.5 MHz, $CDCl_3$, δ_C): 20.1, 21.3, 52.5, 55.0, 103.5 (t, $^2J_{F\text{-}C}$ = 44.9 Hz), 130.1 (t, $^4J_{F\text{-}C}$ = 1.9 Hz), 133.2 (t, $^3J_{F\text{-}C}$ = 14.6 Hz), 134.1, 134.2 (t, $^3J_{F\text{-}C}$ = 8.0 Hz), 135.3;

^{11}B{^{1}H} NMR (96.3 MHz, $CDCl_3$, δ_B): -0.97;

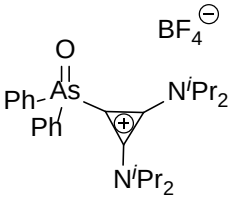
^{19}F{^{1}H} NMR (282.4 MHz, $CDCl_3$, δ_F): -77.8 (s, 2F) -153.31 ($^{10}BF_4$), -153.37 ($^{11}BF_4$);

FT-IR (ν, cm^{-1}): 477, 540, 644, 688, 748, 892, 998, 1048, 1146, 1185, 1355, 1377, 1443, 1457, 1563, 1874, 2938, 2978;

ESI-MS (m/z): 503.2 $[M - BF_4^-]^+$;

HRMS (m/z): calculated for $C_{27}H_{38}As_1F_2N_2$ $[M - BF_4^-]^+$: 503.221332; found: 503.221070 (0.52 ppm).

Synthesis of **29**:



To an argon filled Schlenk flask containing **6** (60.0 mg, 0.109 mmol) and *m*-CPBA (24.3, 0.109 mmol, 77% purity) at room temperature was added CH_2Cl_2 (3 mL) and the reaction mixture was stirred for two hours. At that point Et_2O (10 mL) was added dropwise over a couple minutes, which resulted in the eventual formation of a white precipitate. The solids were allowed to settle, the filtrate was removed by cannula filtration, and the precipitate was washed with Et_2O (3 x 2 mL). Drying the isolated solids *in vacuo* gives the arsine oxide as a colourless powder. The compound is sensitive to water, hydrolyzing to give the protonated cyclopropenium salt and diphenylarsenous acid (Ph_2AsO_2H, as determined by ^{1}H NMR spectroscopy).

Yield: 85%, 52.3 mg, 0.0916 mmol;
^{1}H NMR (400 MHz, $CDCl_3$, δ_H): 1.04 (d, 12H, $^{3}J_{H\text{-}H}$ = 6.8 Hz), 1.37 (d, 12H, $^{3}J_{H\text{-}H}$ = 6.8 Hz), 3.49 (sept, 2H, $^{3}J_{H\text{-}H}$ = 6.8 Hz), 4.14 (sept, 2H, $^{3}J_{H\text{-}H}$ = 6.8 Hz), 7.62-7.68 (m, 6H), 8.05-8.10 (m, 4H);
^{13}C{^{1}H} NMR (100.5 MHz, $CDCl_3$, δ_C): 20.3, 21.3, 53.1, 54.3, 99.6, 130.3, 131.0, 131.5, 133.6, 139.1;
^{11}B{^{1}H} NMR (96.3 MHz, $CDCl_3$, δ_B): -0.99;
^{19}F{^{1}H} NMR (282.4 MHz, $CDCl_3$, δ_F): -151.50 ($^{10}BF_4$), -151.54 ($^{11}BF_4$);
FT-IR (ν, cm^{-1}): 457, 520, 579, 637, 692, 757, 906, 999, 1048, 1148, 1349, 1377, 1441, 1460, 1566, 1590, 1865, 2937;
ESI-MS (m/z): 481.3 $[M - BF_4^-]^+$;
HRMS (m/z): calculated for $C_{27}H_{38}As_1N_2O_1$ $[M - BF_4^-]^+$: 481.219440; found: 481.219370 (0.15 ppm).

Platinum Catalysis:

A 1,2-DCE solution of the substrate (25 mg, 0.086 mmol), internal standard tridecane (16 mg, 21 μL, 0.086 mmol), and the trichloroplatinate arsine compounds (5 mol%) at 80 °C were treated with a 1,2-DCE solution of $AgSbF_6$ (5 mol%), to give an overall concentration of 0.1 M.

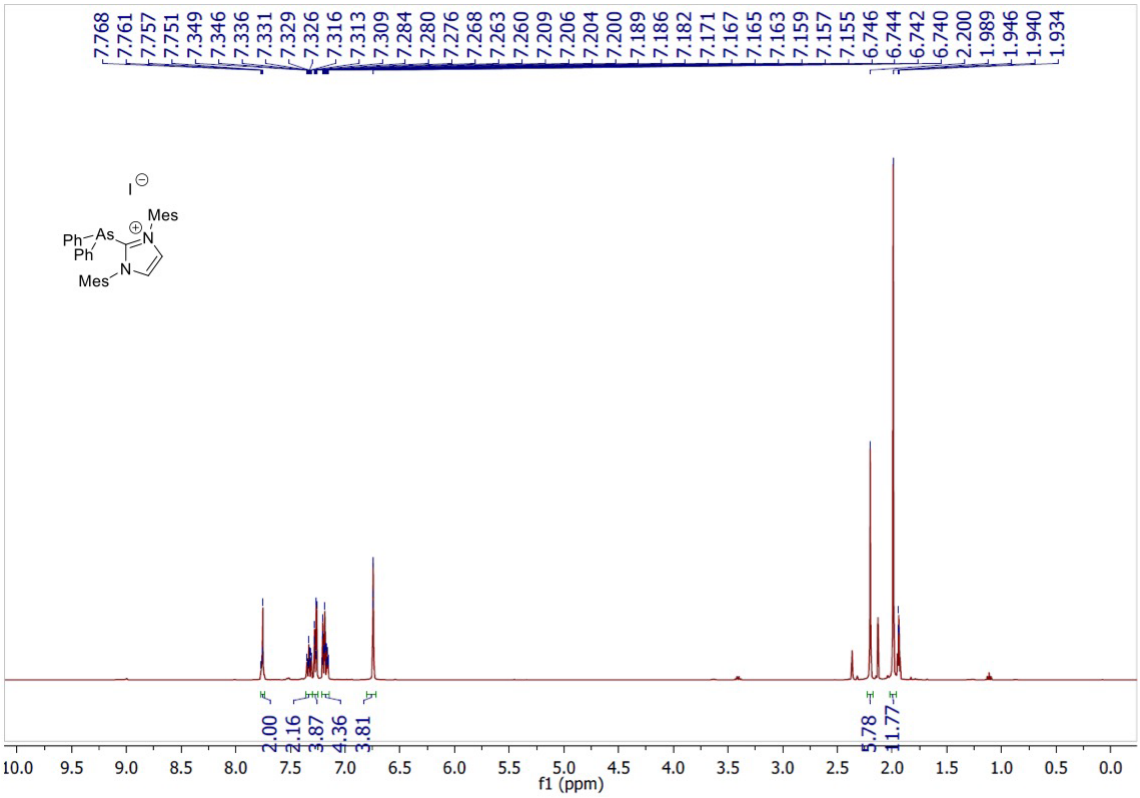
The catalysts involving neutral ligands were generated *in situ* by adding 1,2-DCE to a mixture of substrate (25 mg, 0.086 mmol), internal standard tridecane (16 mg, 21 μL, 0.086 mmol), neutral ligand (5 mol%), and $PtCl_2$ (5 mol%) at 80 °C, to give an overall concentration of 0.1 M.

Samples were taken at regular time intervals, filtered through a plug of silica using dichloromethane and their GC chromatographs were recorded. Conversion was measured as the consumption of starting material relative to the internal standard. After the reaction was over the mixture was filtered over a plug of silica using dichloromethane, and the solvent was removed *in vacuo*. Analysis of this crude residue by ^1H NMR spectroscopy reveals a product/standard ratio similar to the original starting material/standard.

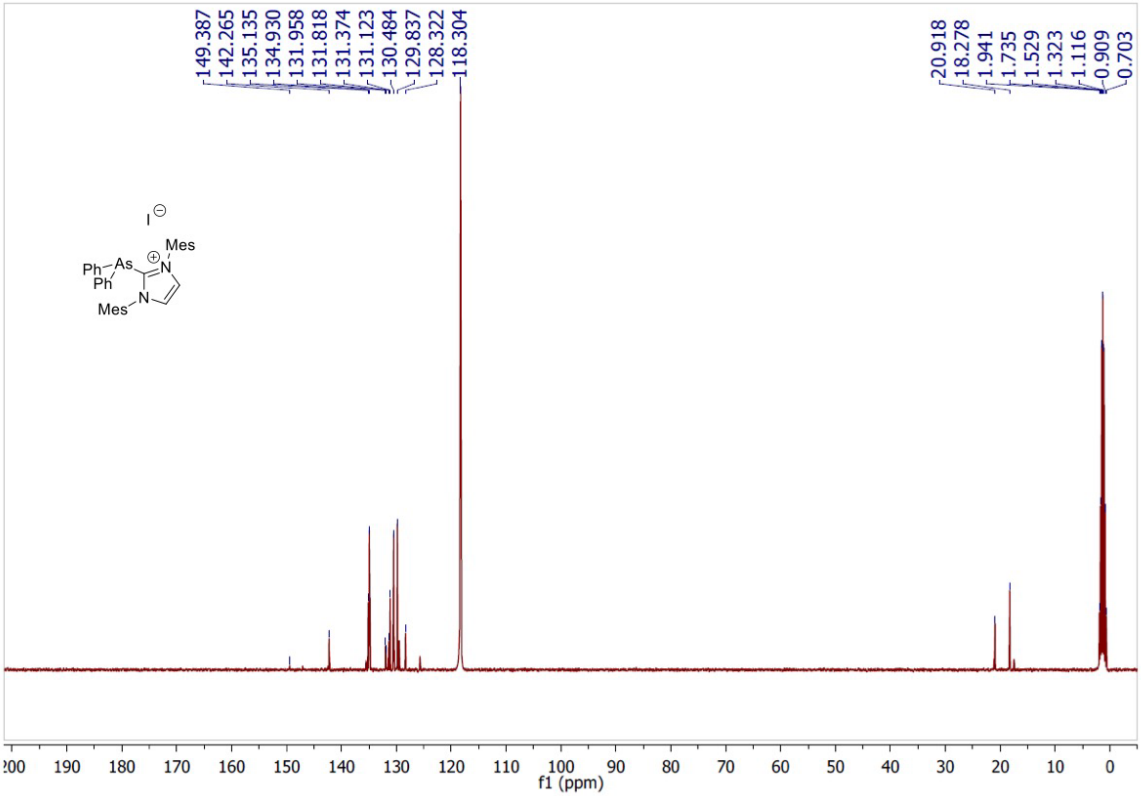
In order to isolate the major product, the reaction was performed with 75 mg of substrate (0.259 mmol) and the catalyst was generated using $AgSbF_6$ (4.45 mg, 0.013 mmol, 0.05 equiv) and **21.** After 30 minutes the reaction was filtered through a plug of silica and the volatile components were removed *in vacuo*. The product was isolated after flash silica gel chromatography using a 92:8 pentane:ethylacetate mixture as the eluent (Rf = 0.28). A colourless oil was obtained, which solidified upon storage at 4 °C (75%, 56.7 mg, 0.196 mmol). The identity of the product was confirmed by comparison of the ^1H and $^{13}C\{^1H\}$ NMR spectra to the literature (previously isolated in only 12% yield).[13] Single crystals suitable for structural determination analysis were grown from a saturated pentane solution with 3 drops of Et_2O at 4 °C.

3) Selected NMR Spectra of New Compounds

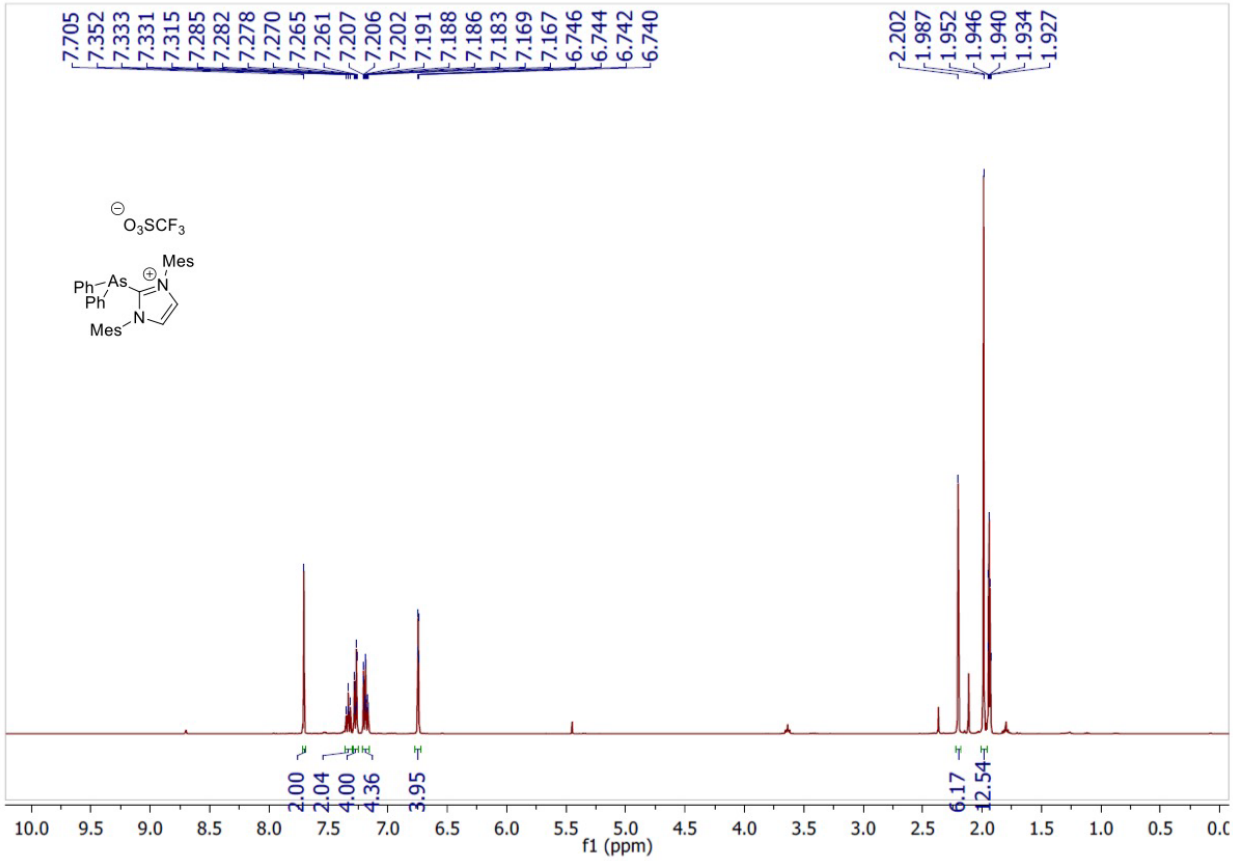
^{1}H-NMR of **2**



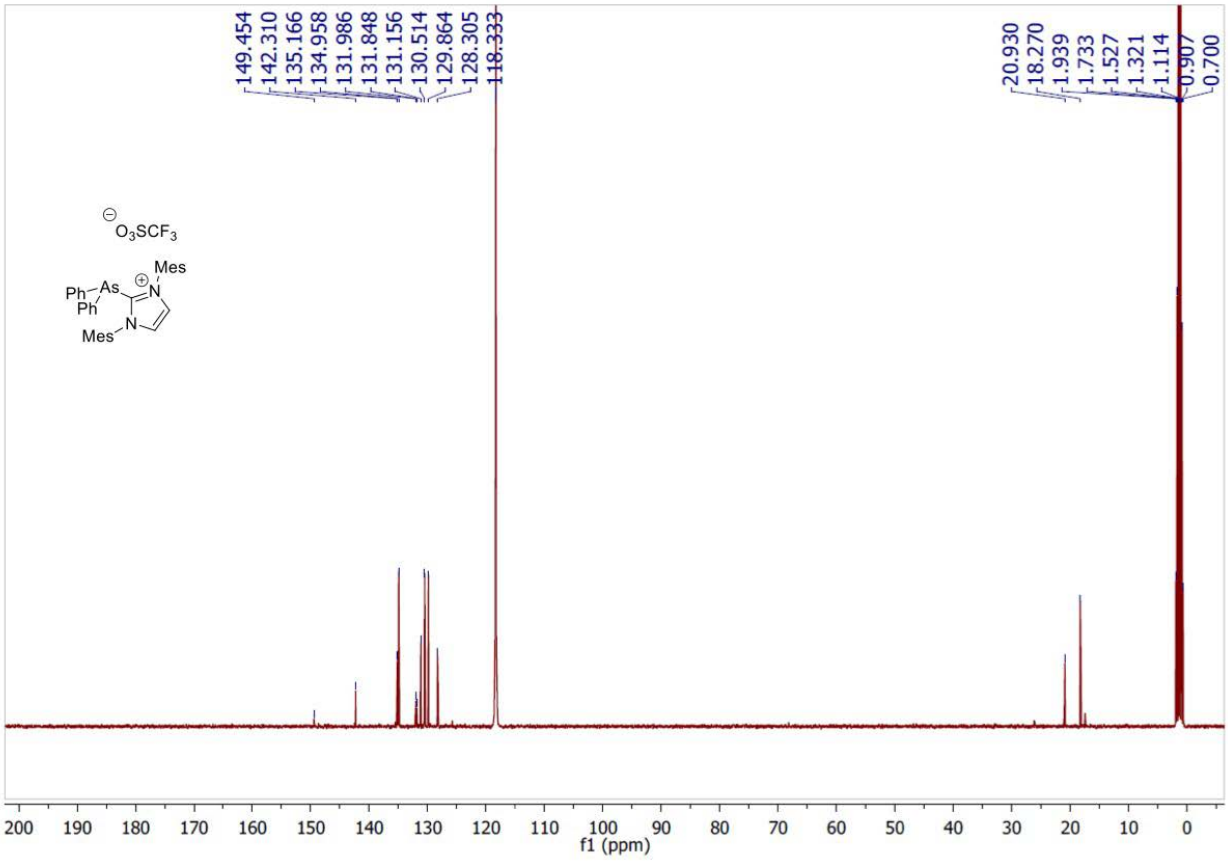
^{13}C-NMR of **2**



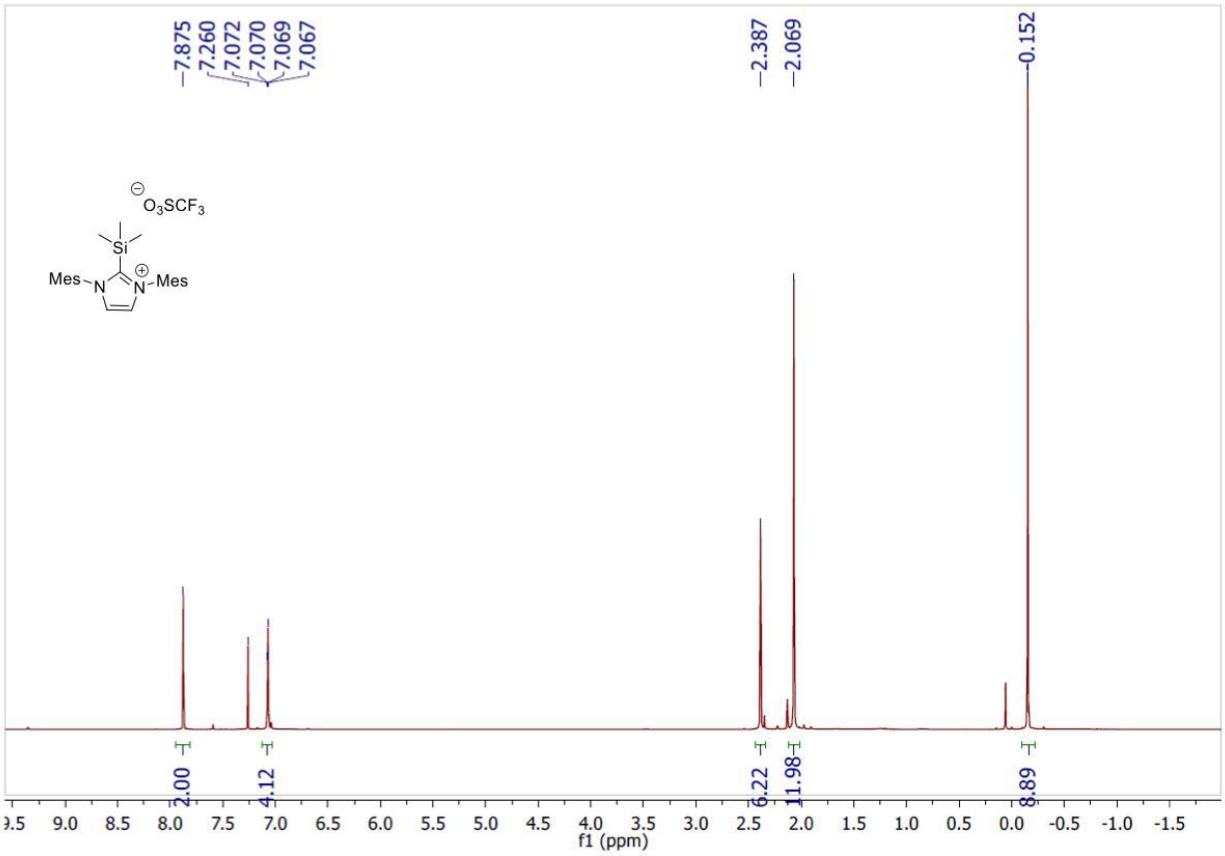
^{1}H-NMR of **3**



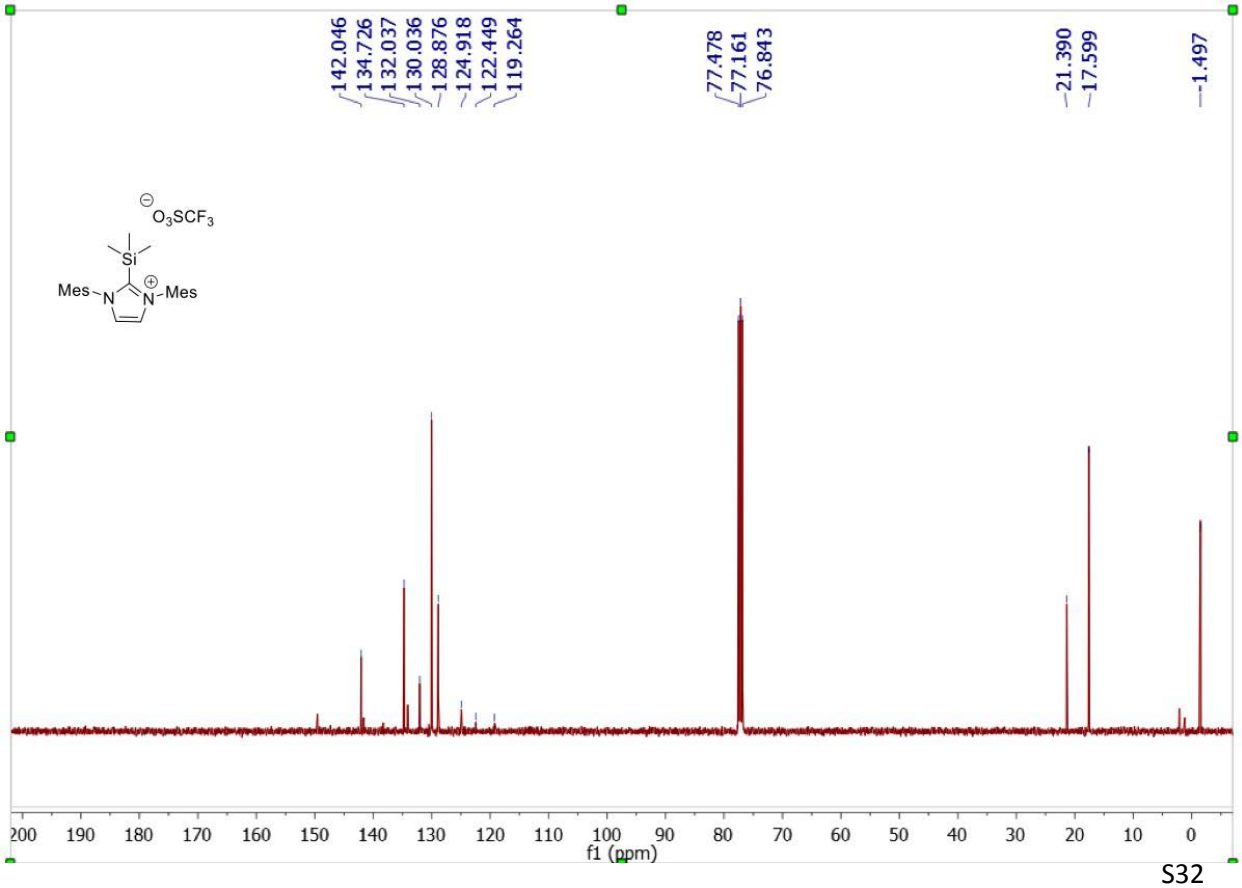
^{13}C-NMR of **3**



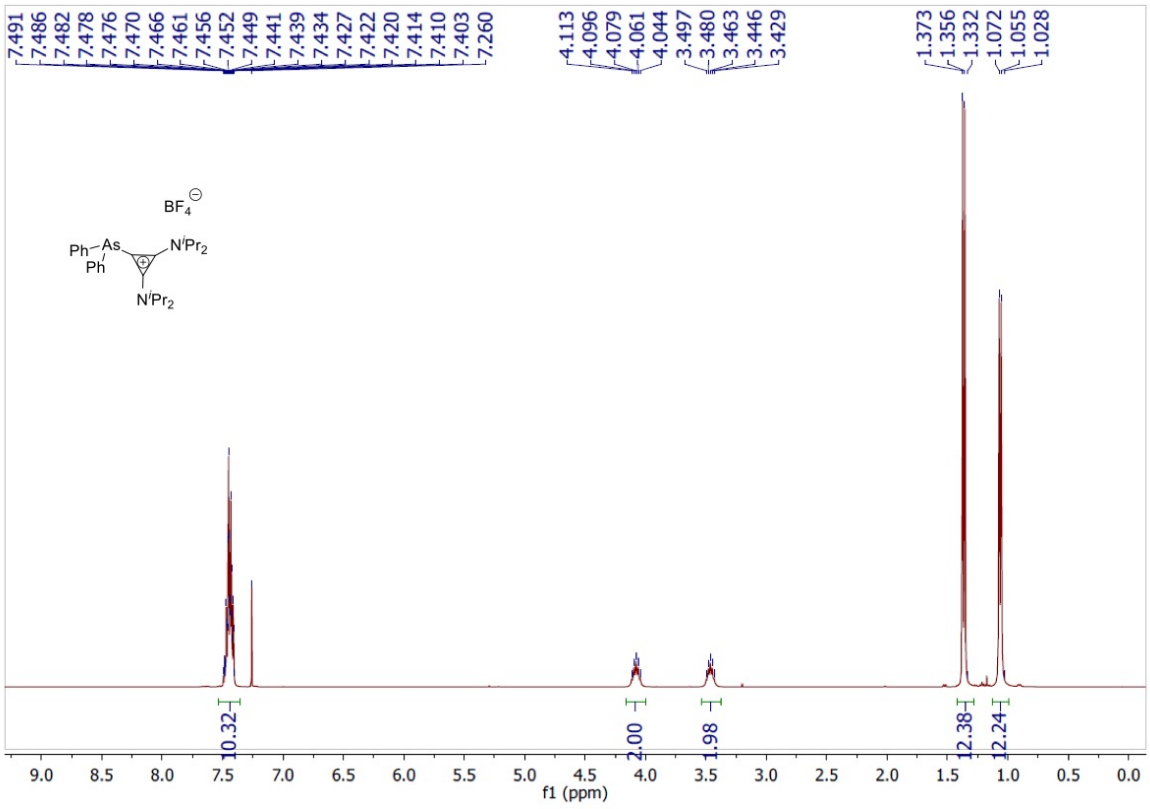
^{1}H-NMR of **4**



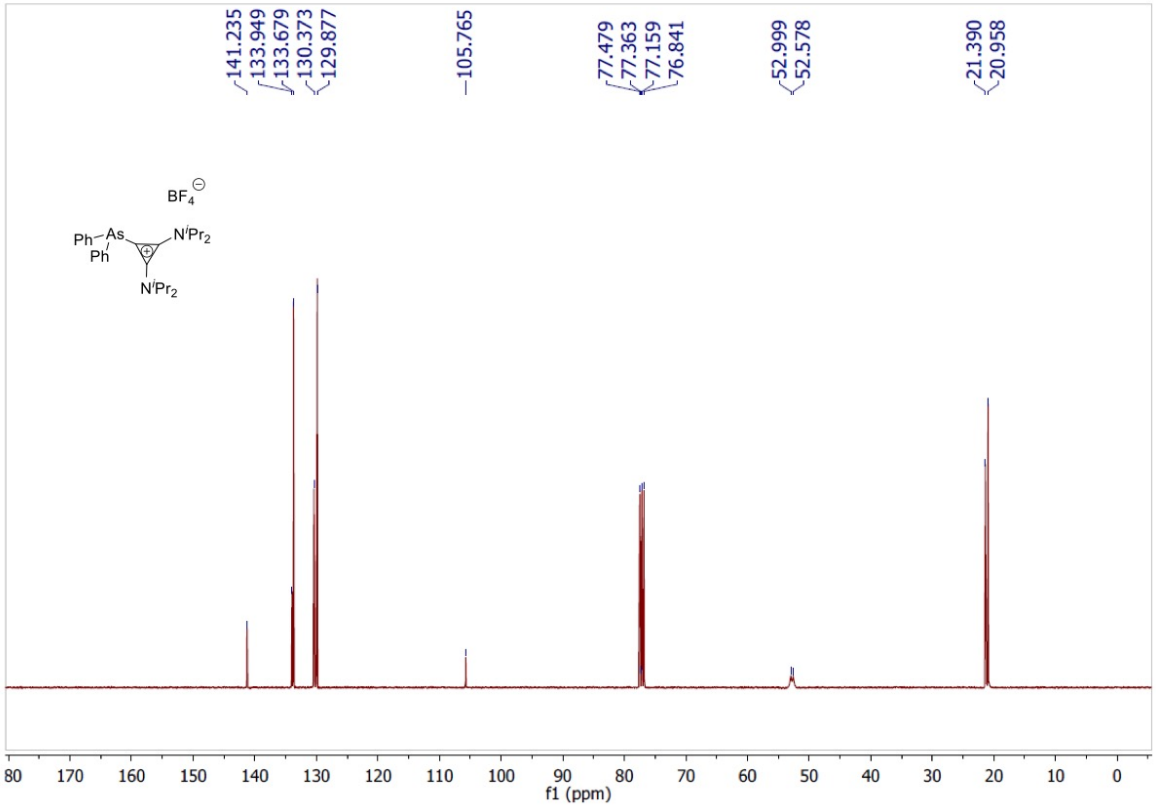
^{13}C-NMR of **4**



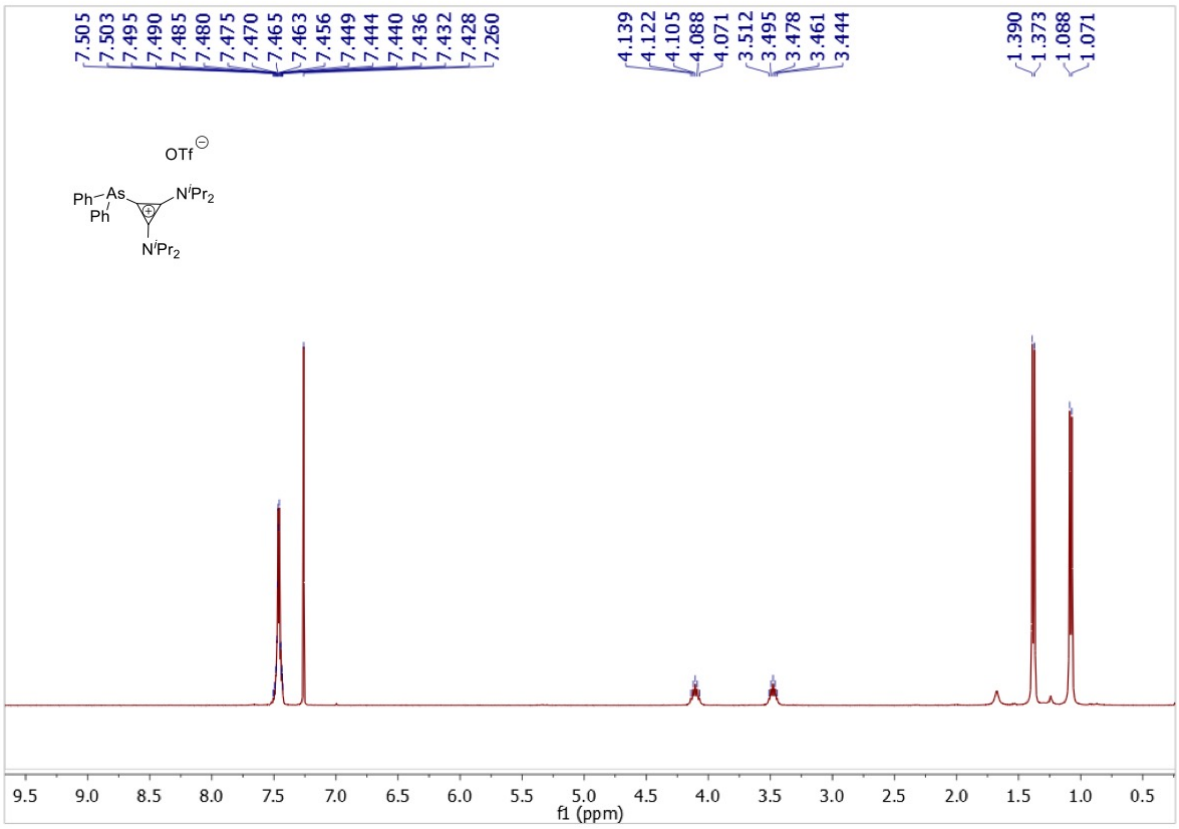
^{1}H-NMR of **6**



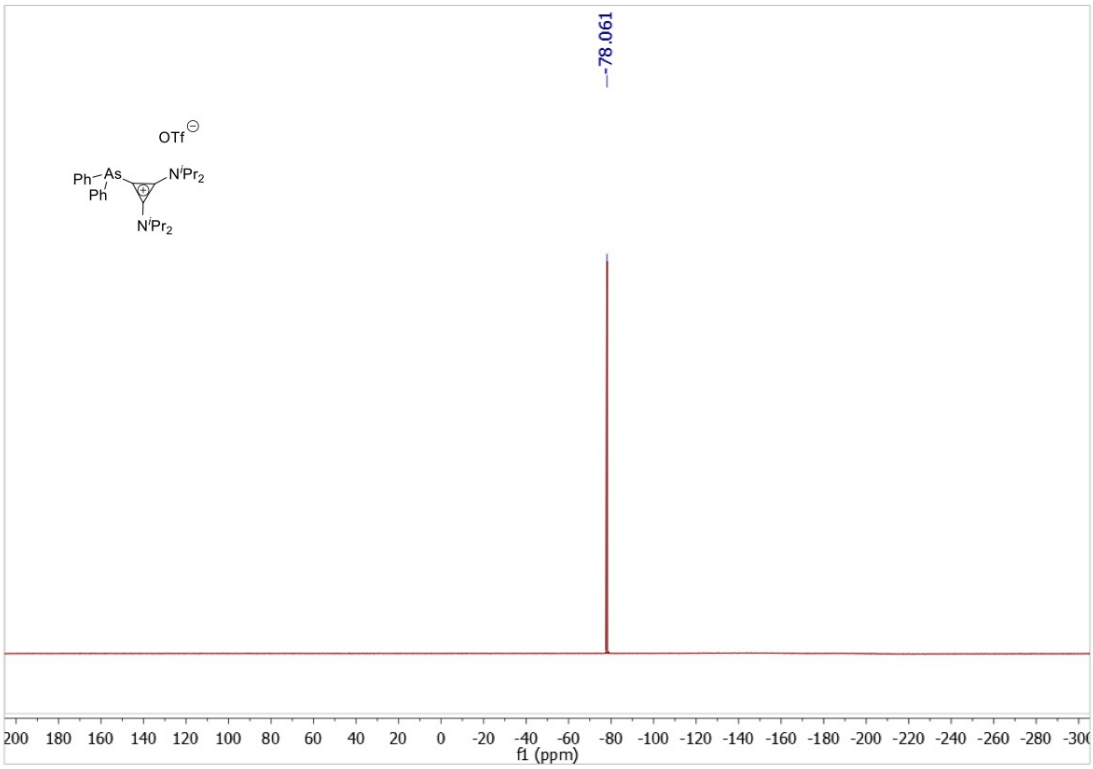
^{13}C-NMR of **6**



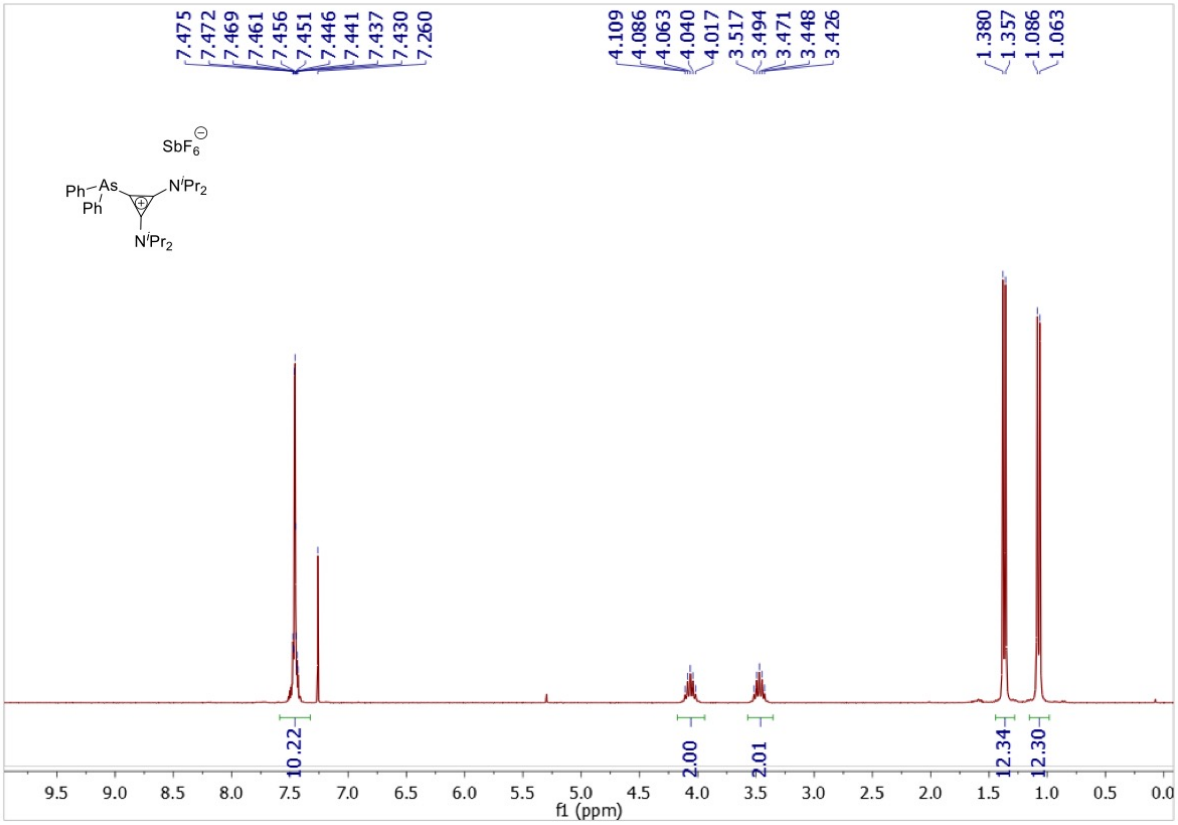
^{1}H-NMR of **7**



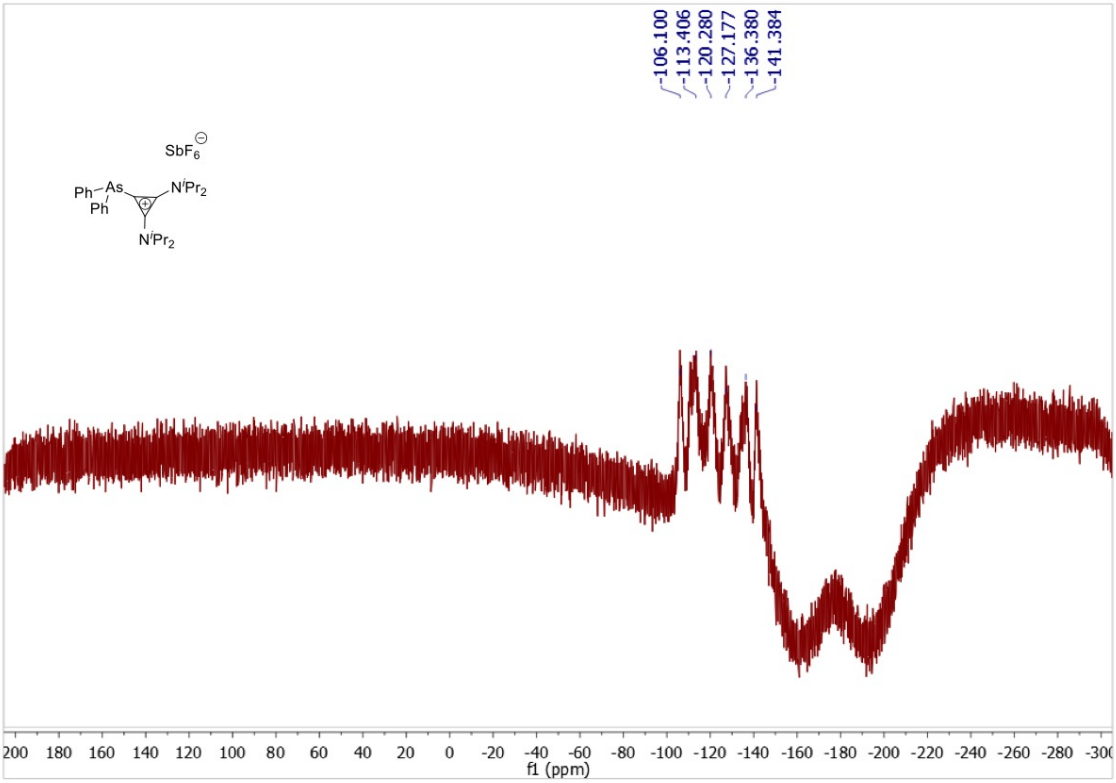
^{19}F-NMR of **7**



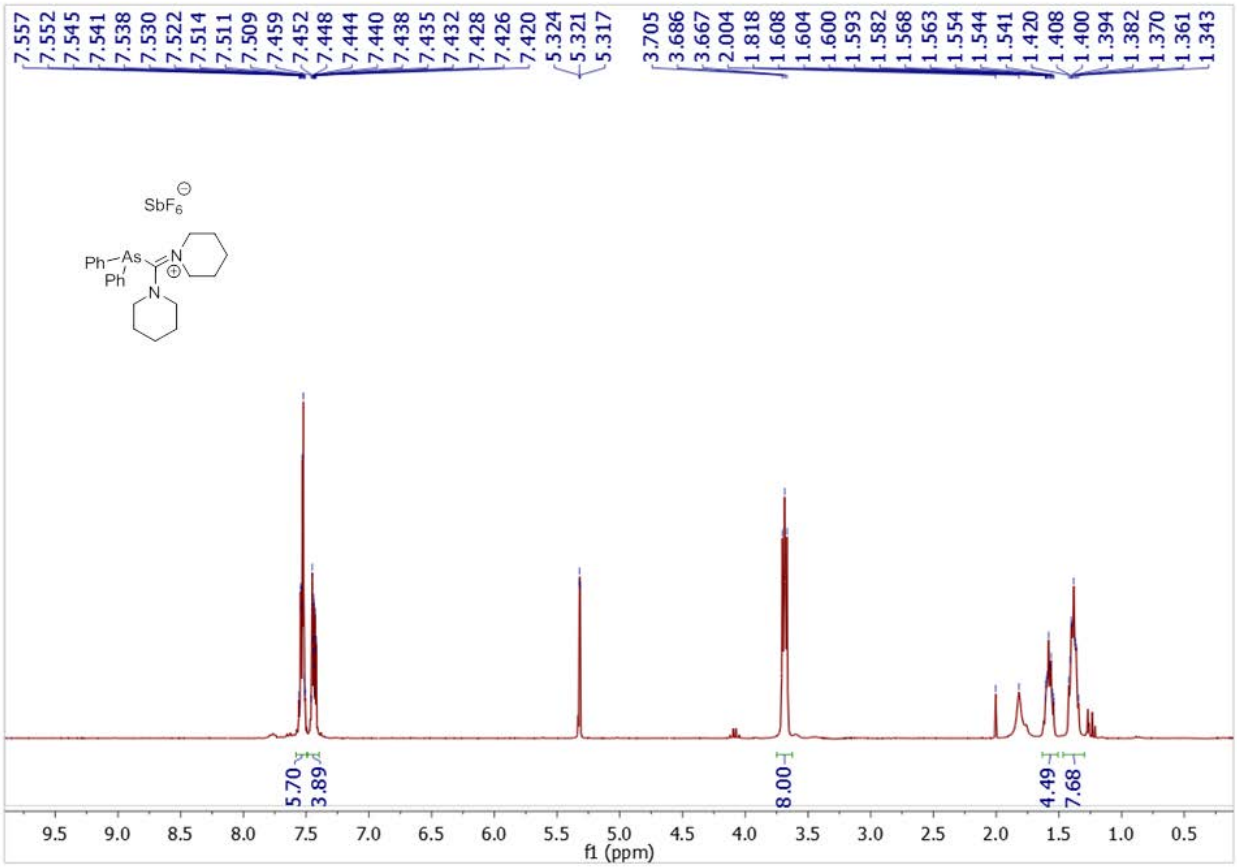
^{1}H-NMR of **8**



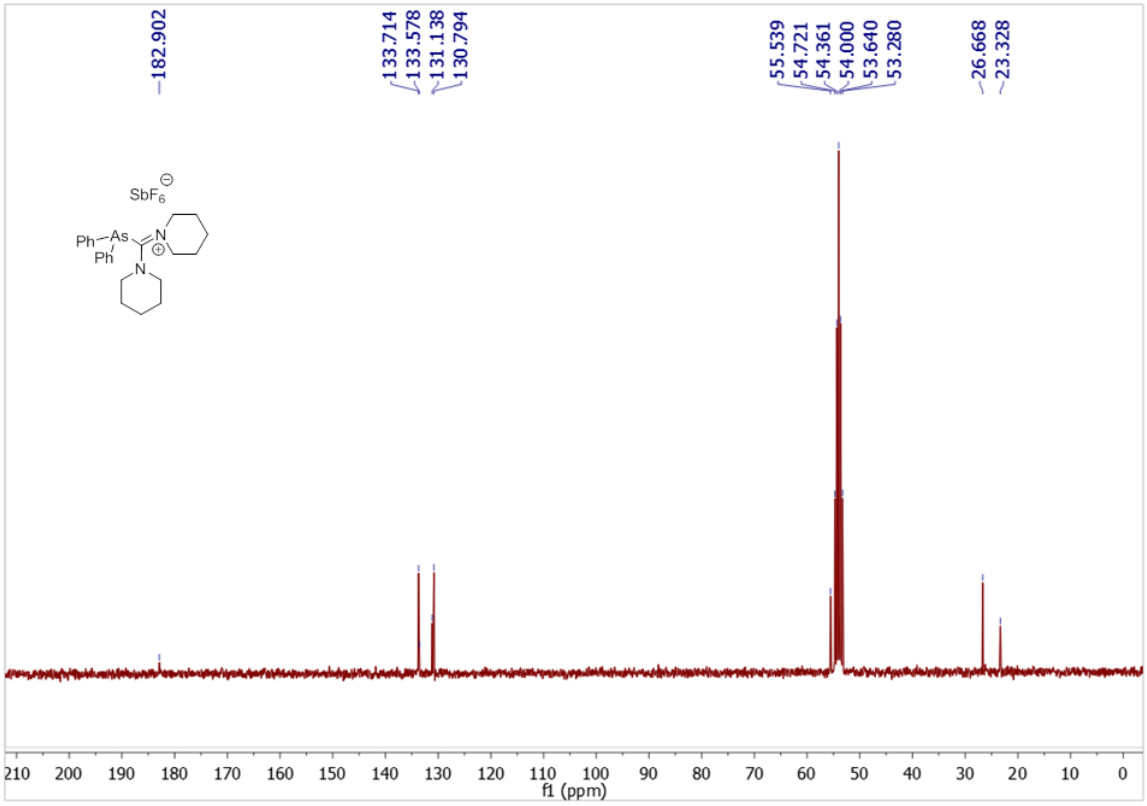
^{19}F-NMR of **8**



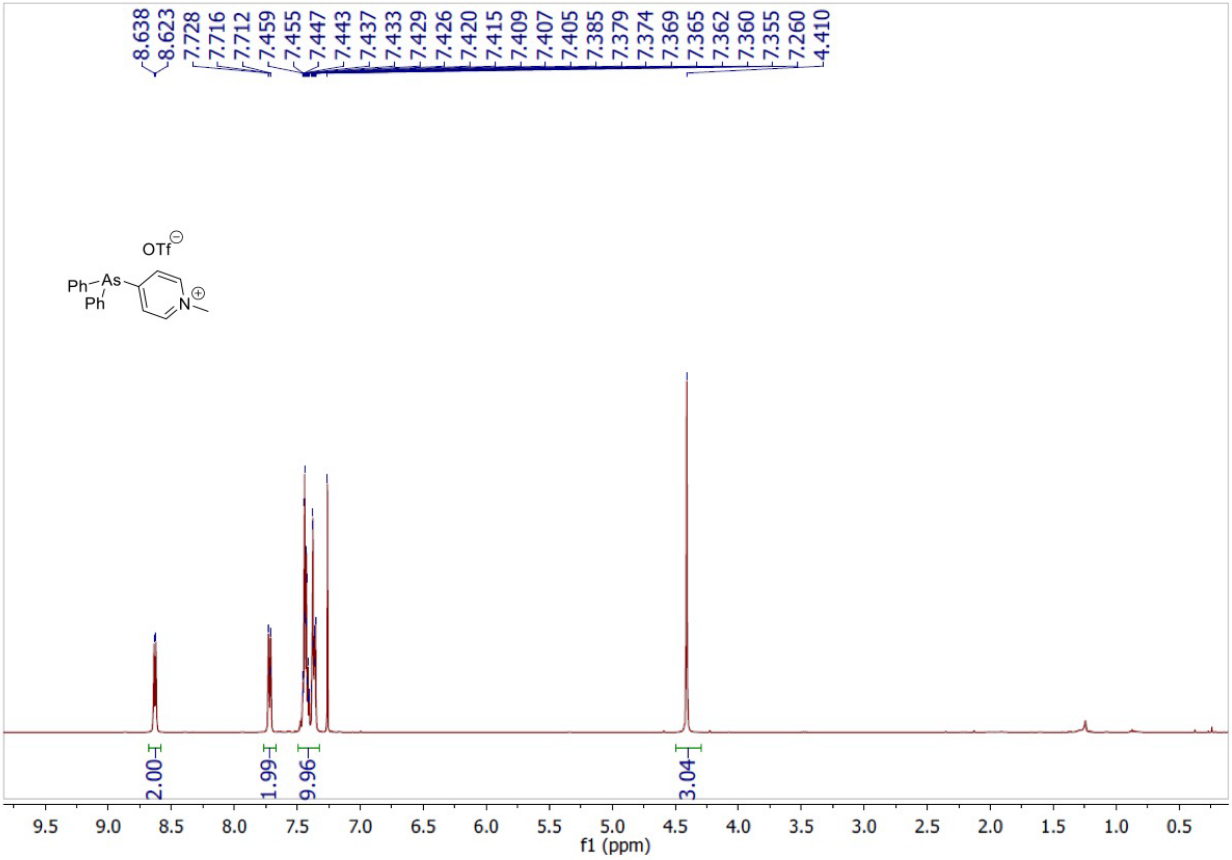
^{1}H-NMR of **9**



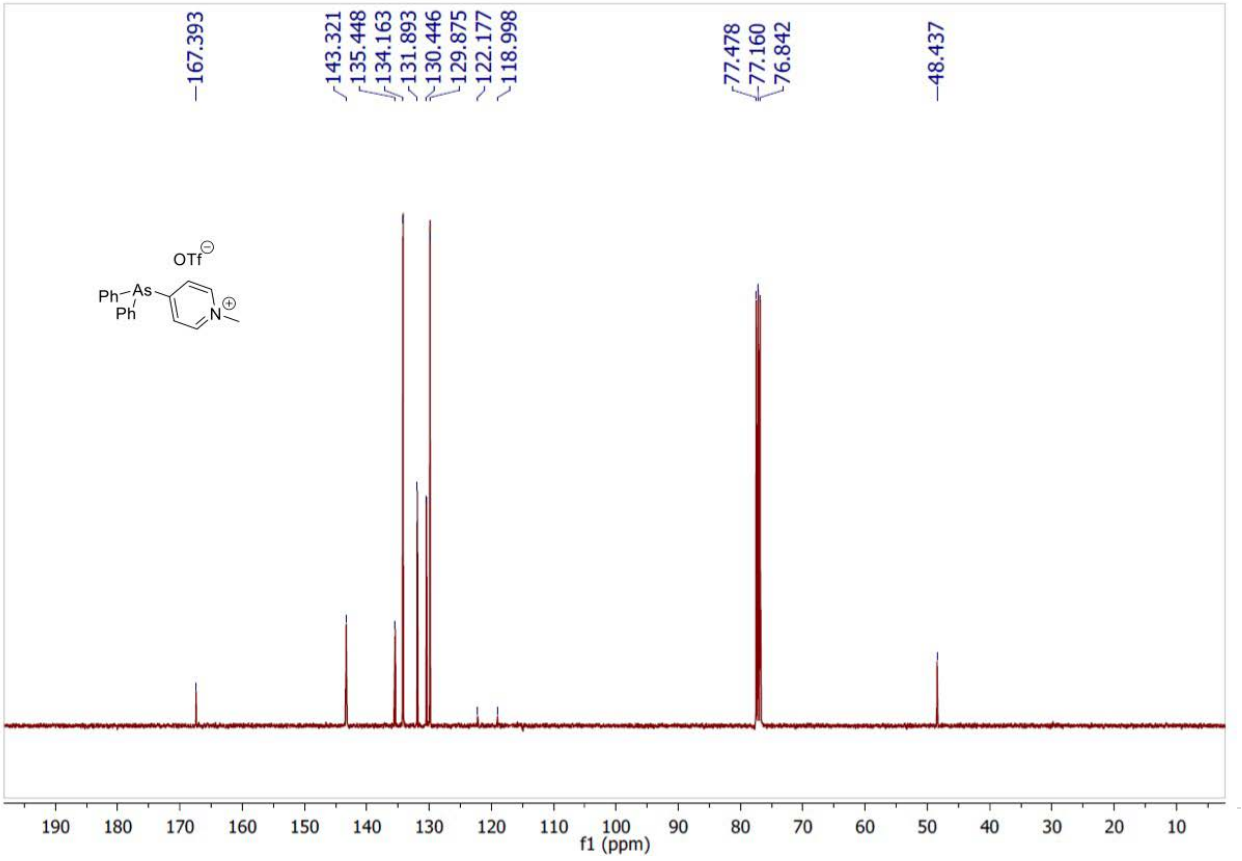
^{13}C-NMR of **9**



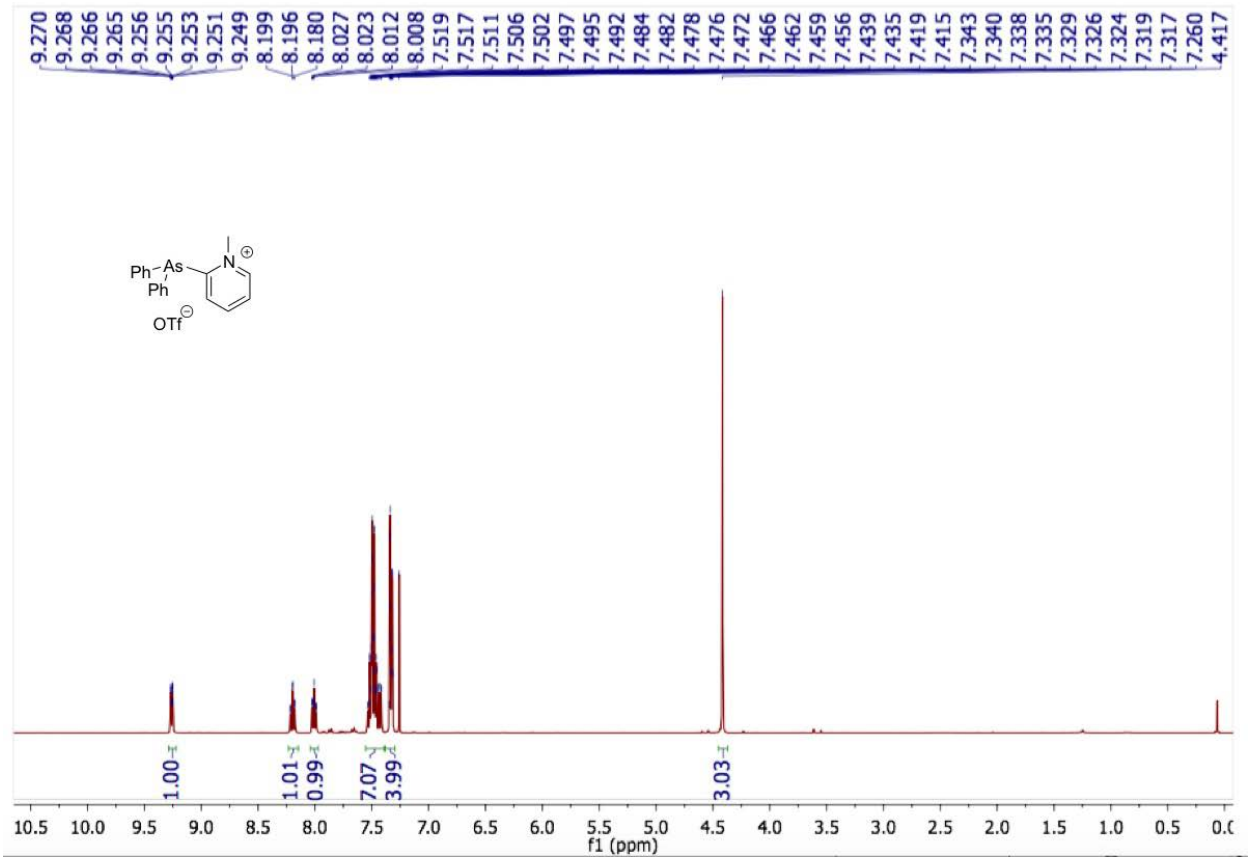
^{1}H-NMR of **10**



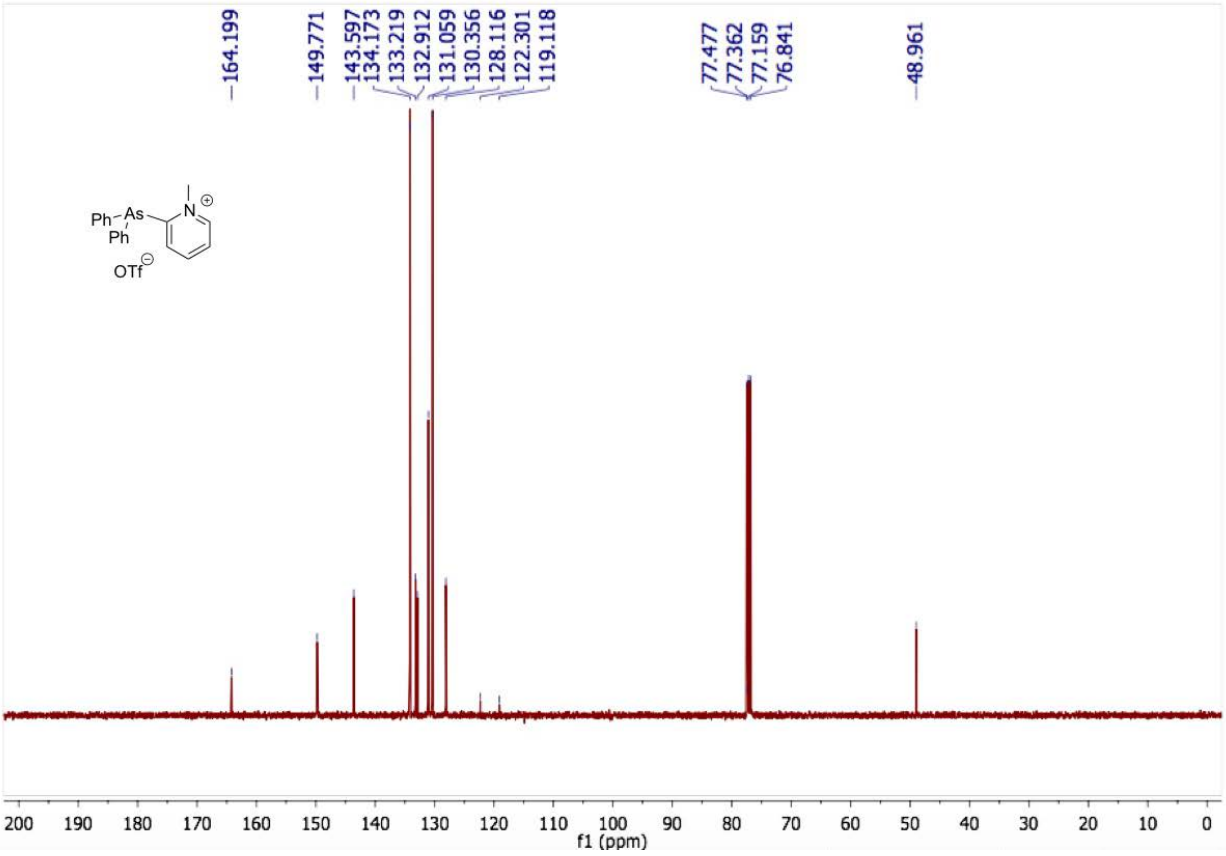
^{13}C-NMR of **10**



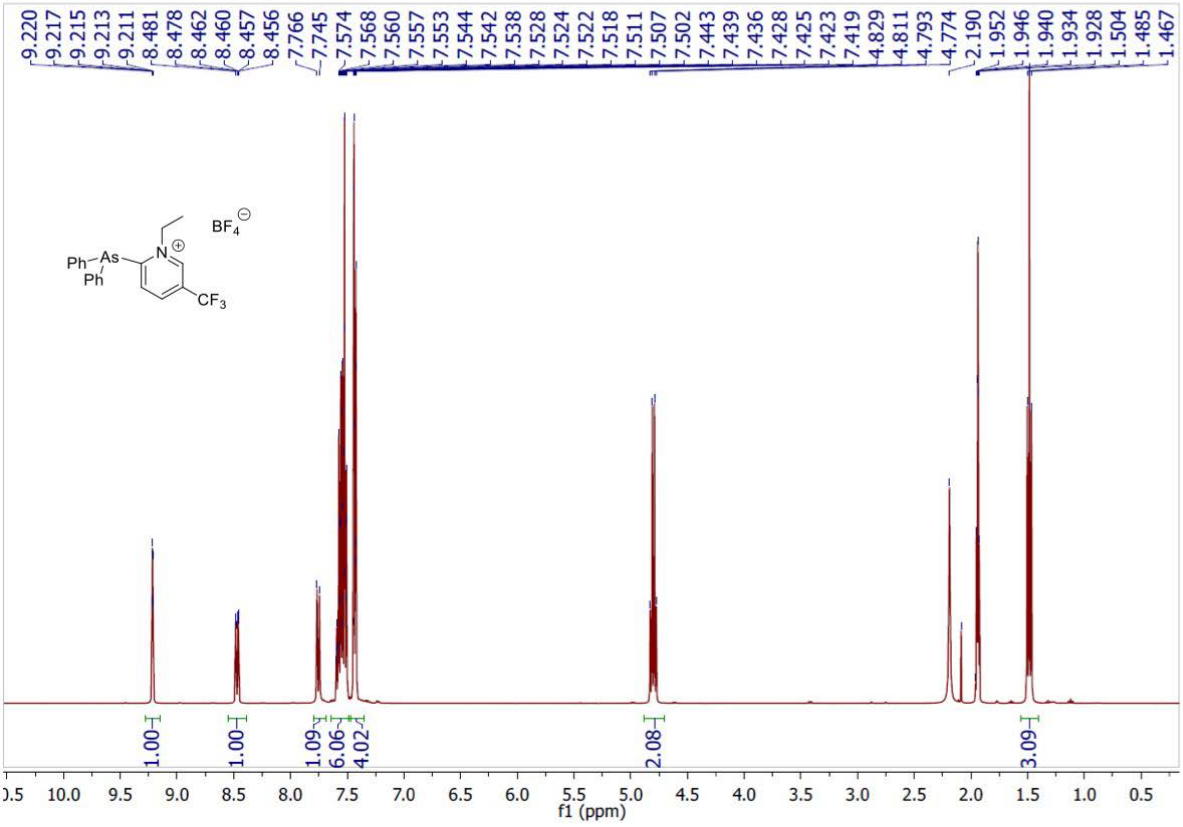
^{1}H-NMR of **11**



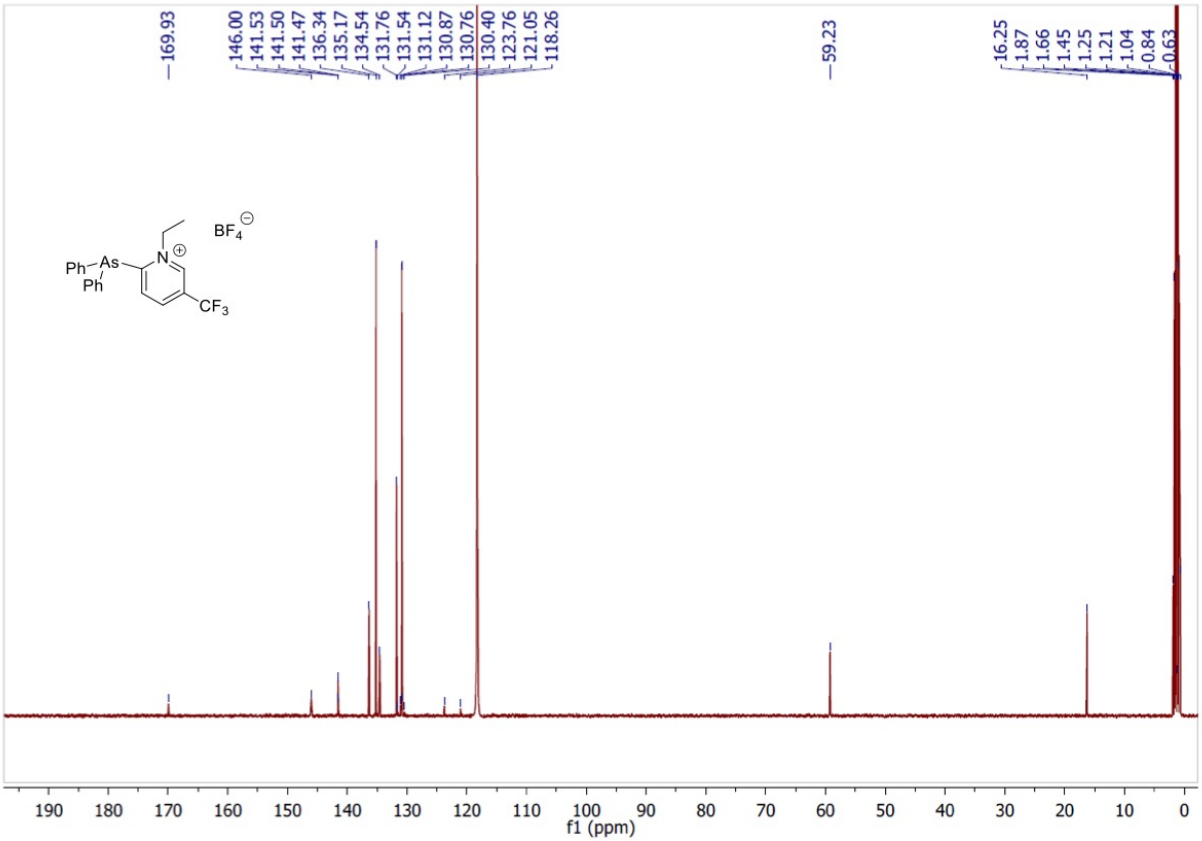
^{13}C-NMR of **11**



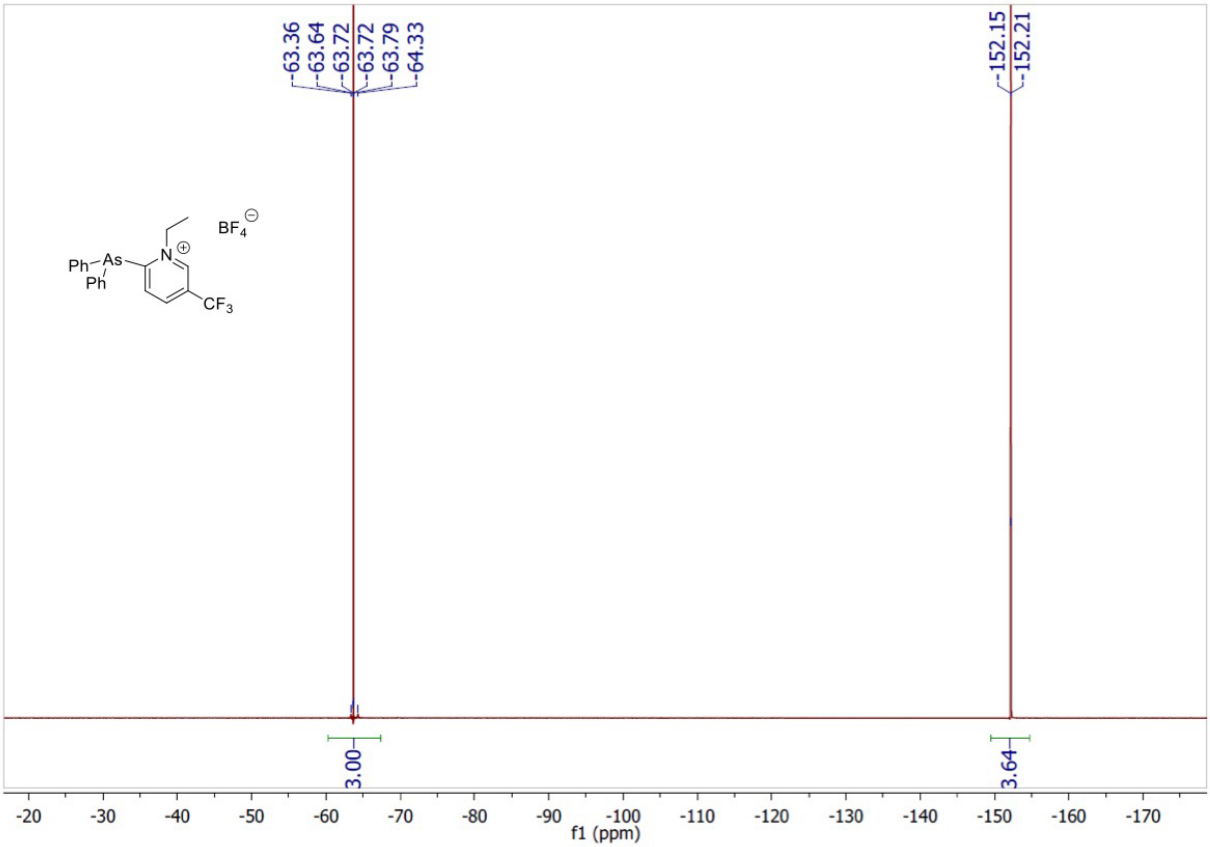
^{1}H-NMR of **13**



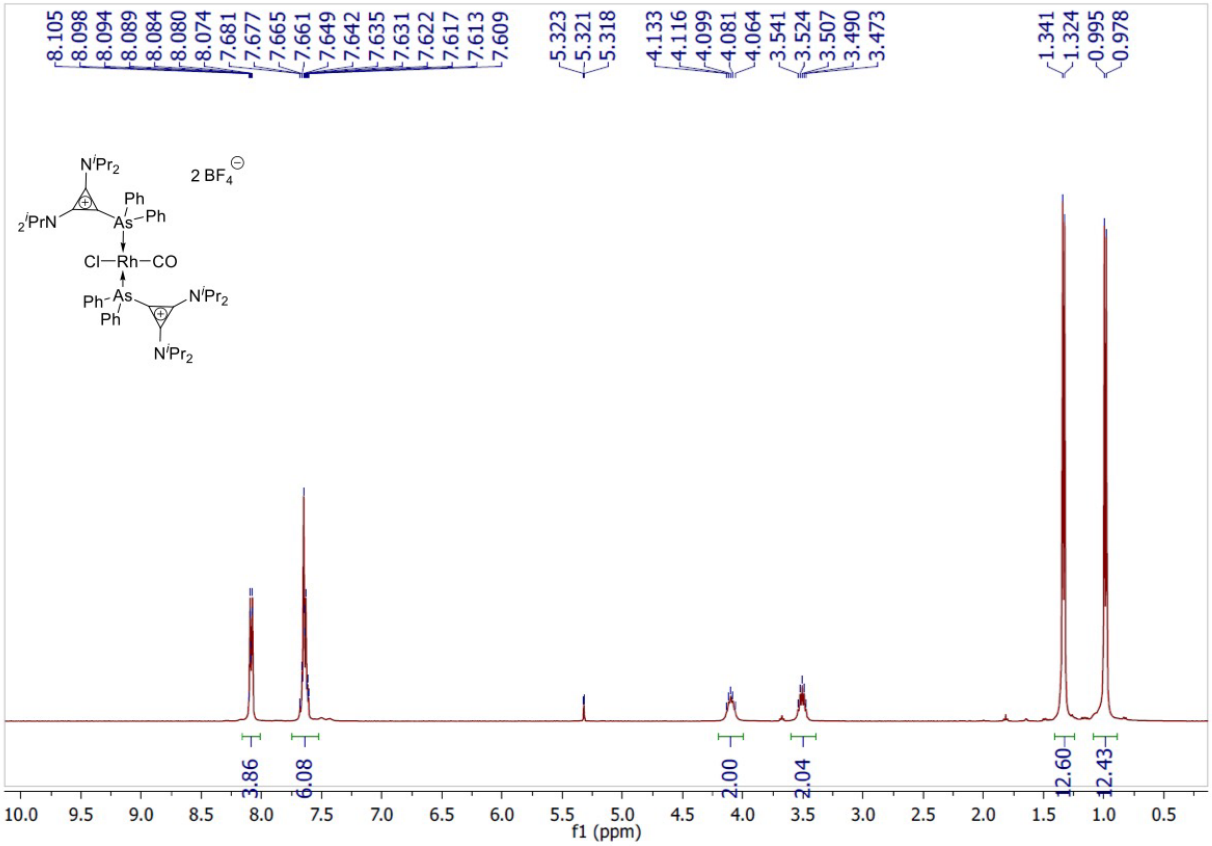
^{13}C-NMR of **13**



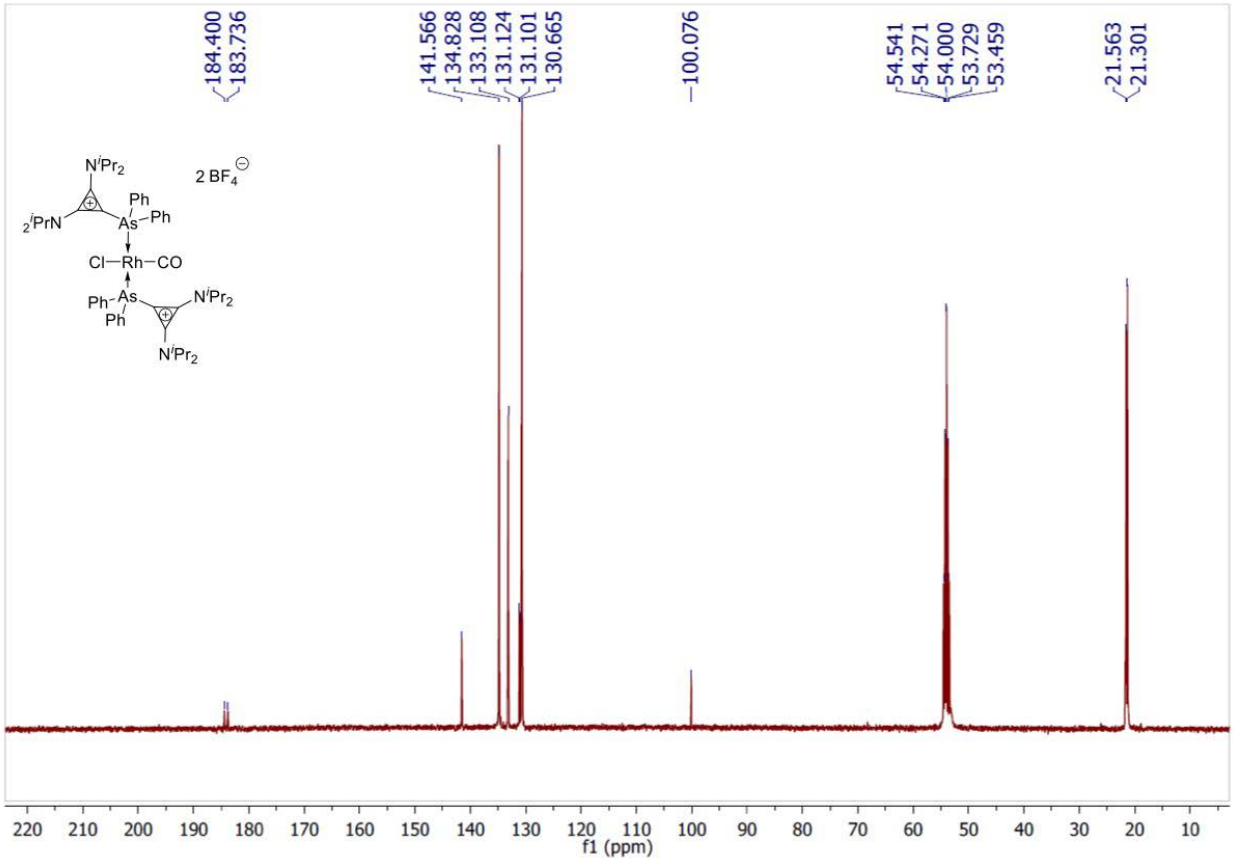
^{19}F-NMR of **13**



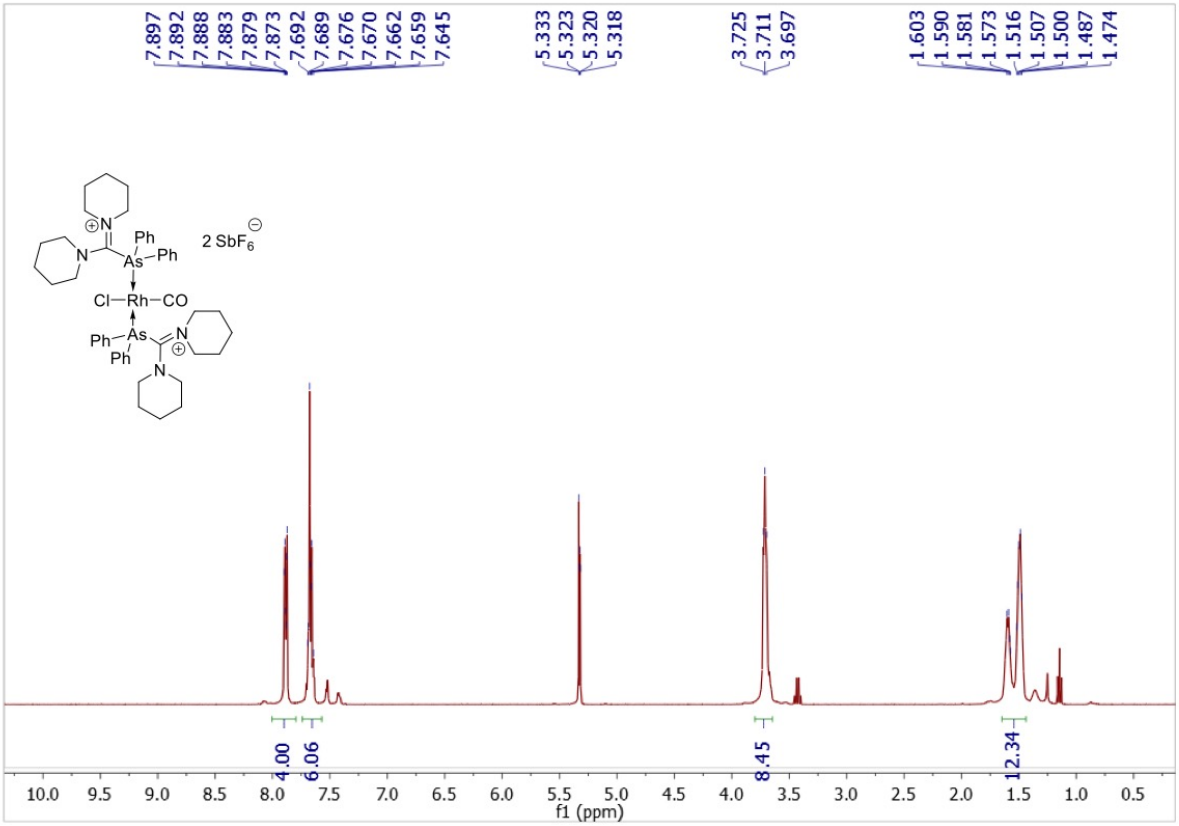
^{1}H-NMR of **14**



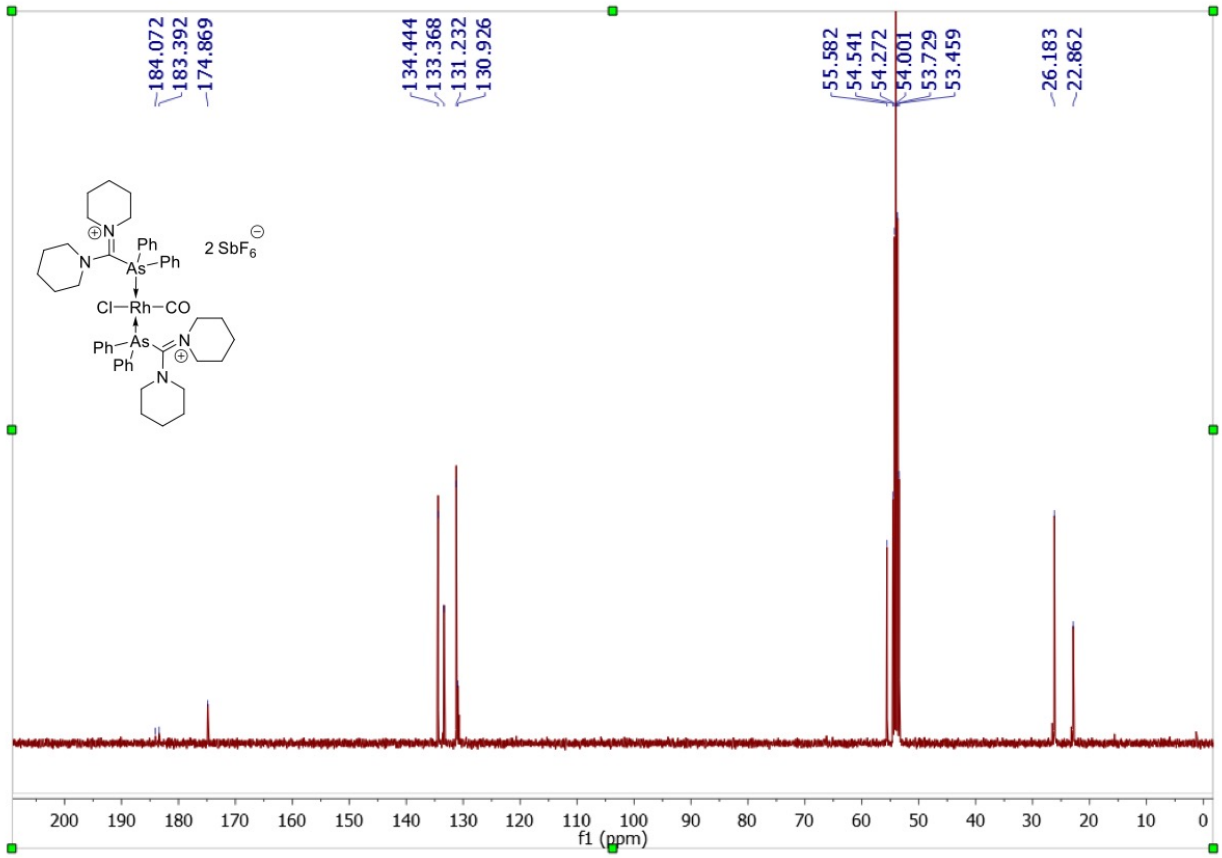
^{13}C-NMR of **14**



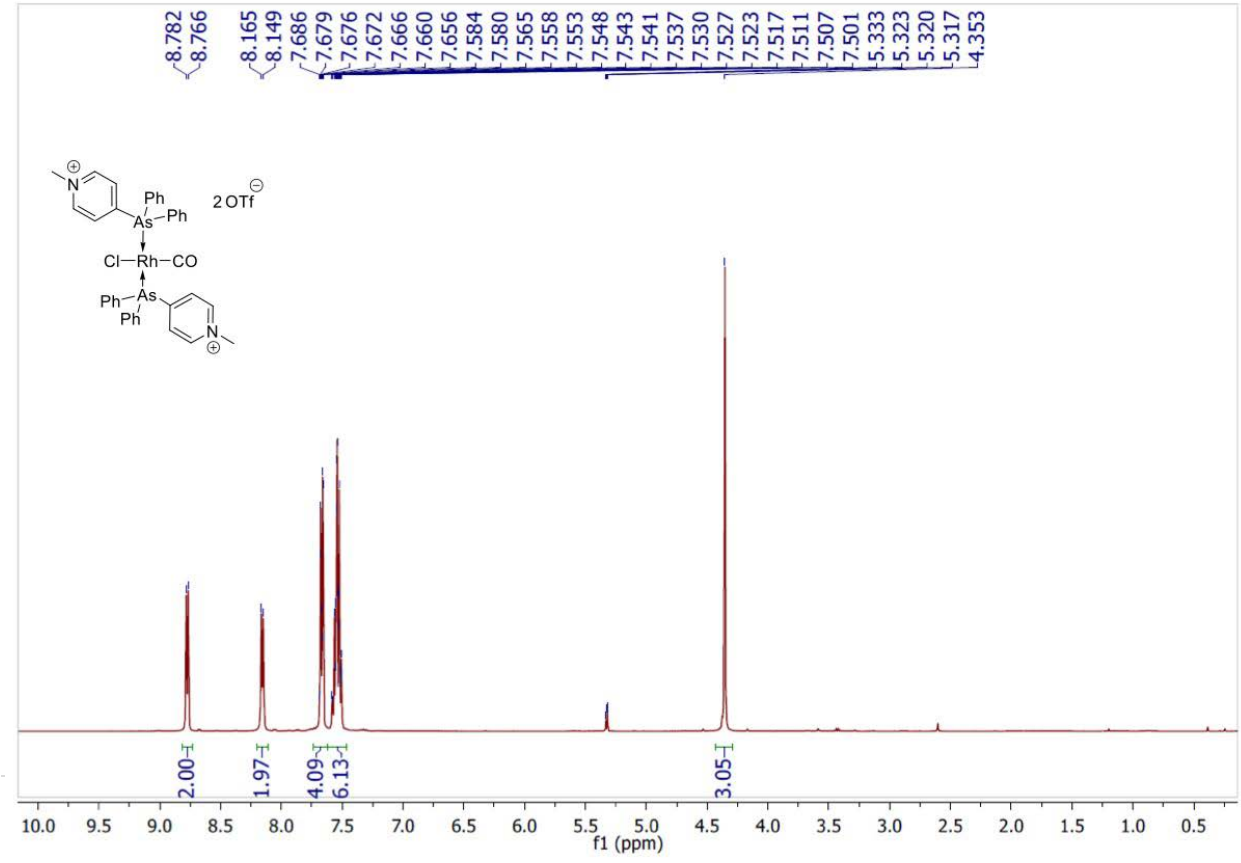
^{1}H-NMR of **15**



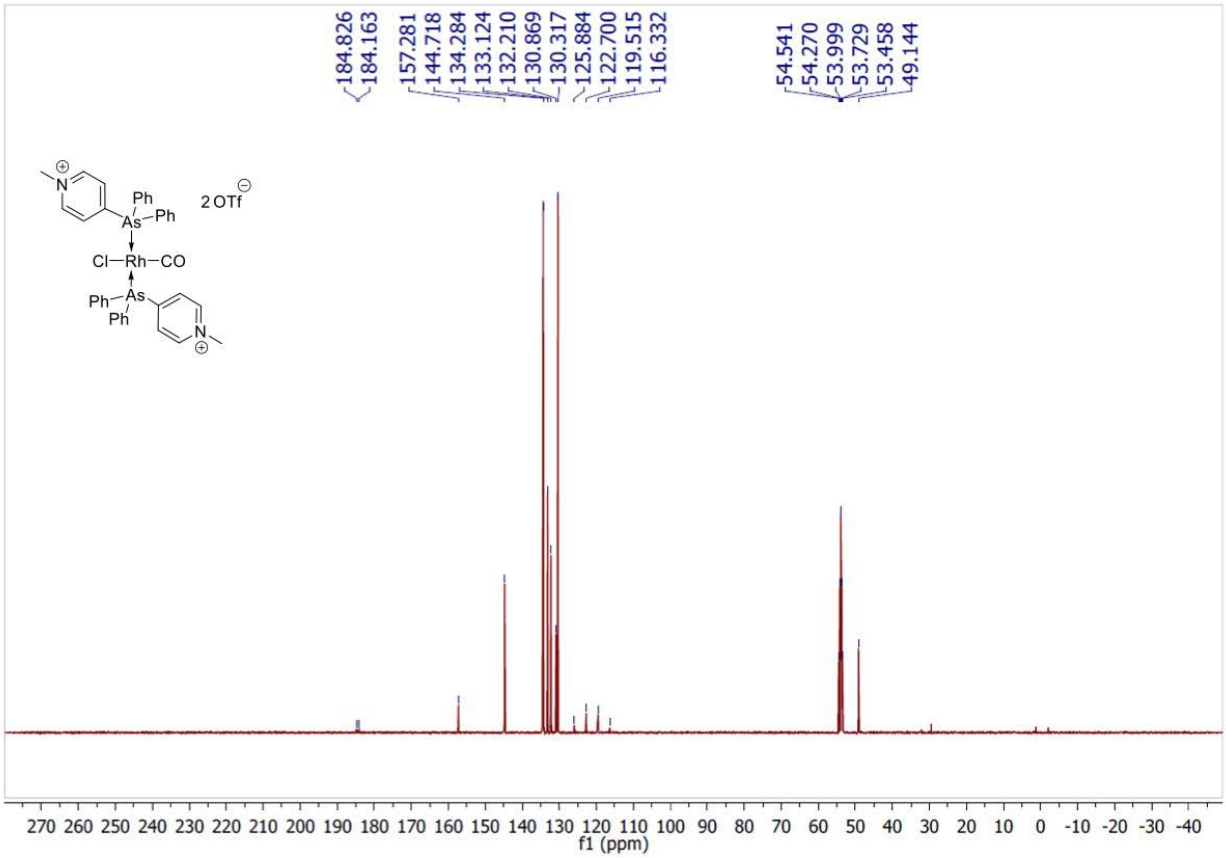
^{13}C-NMR of **15**



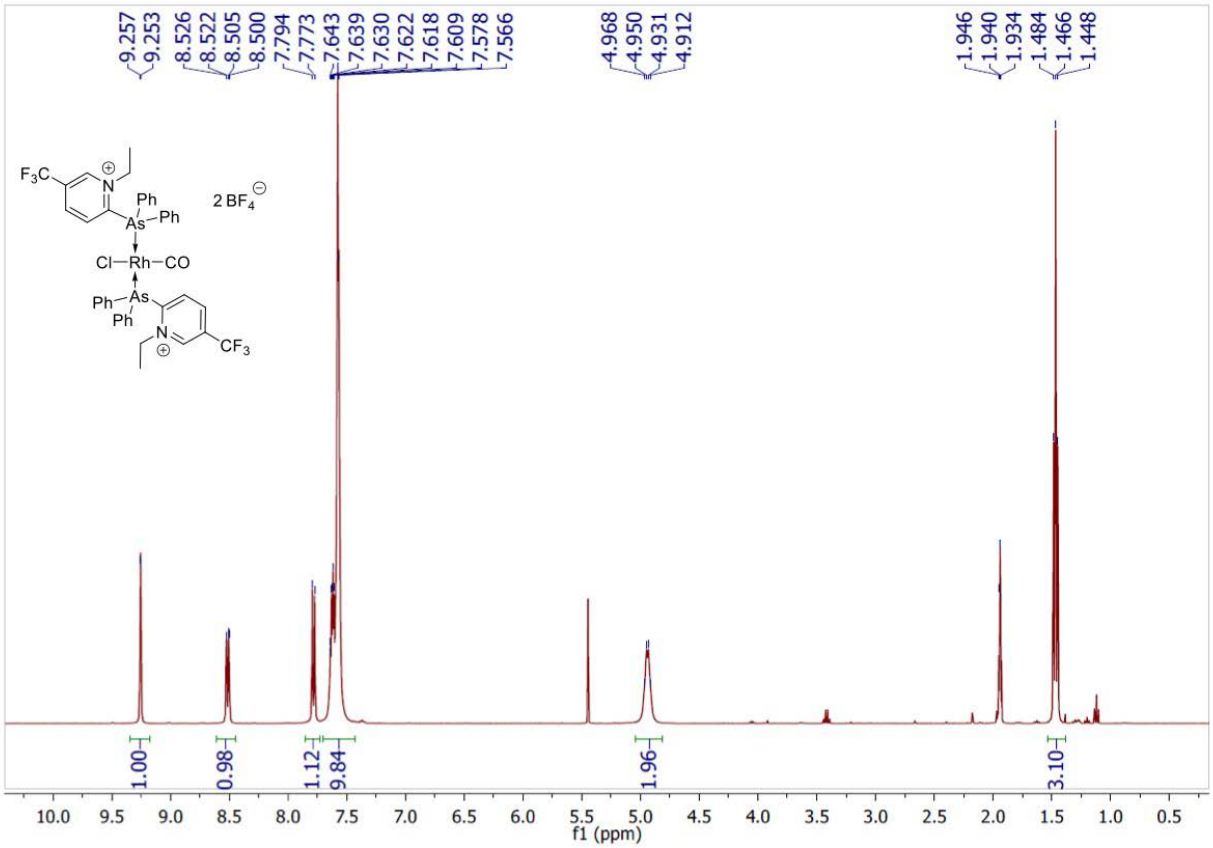
^{1}H-NMR of **16**



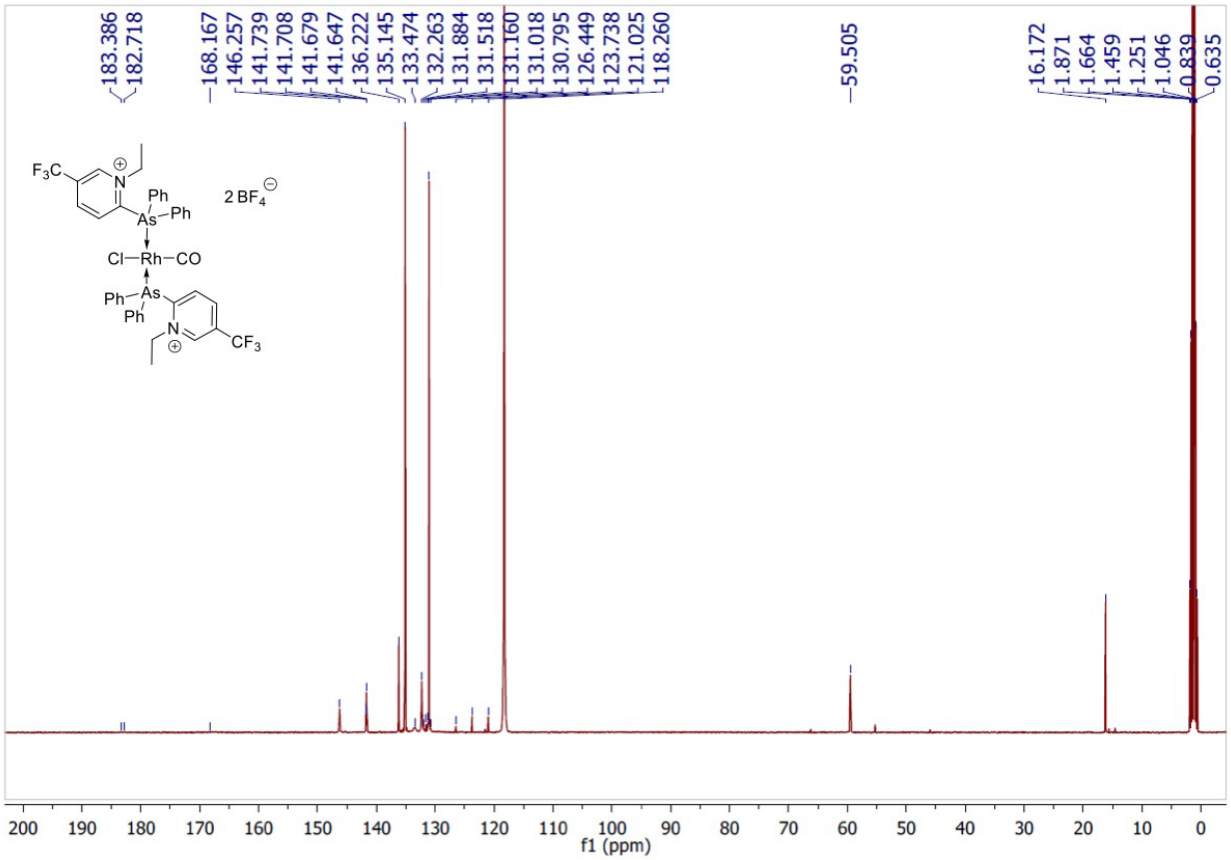
^{13}C-NMR of **16**



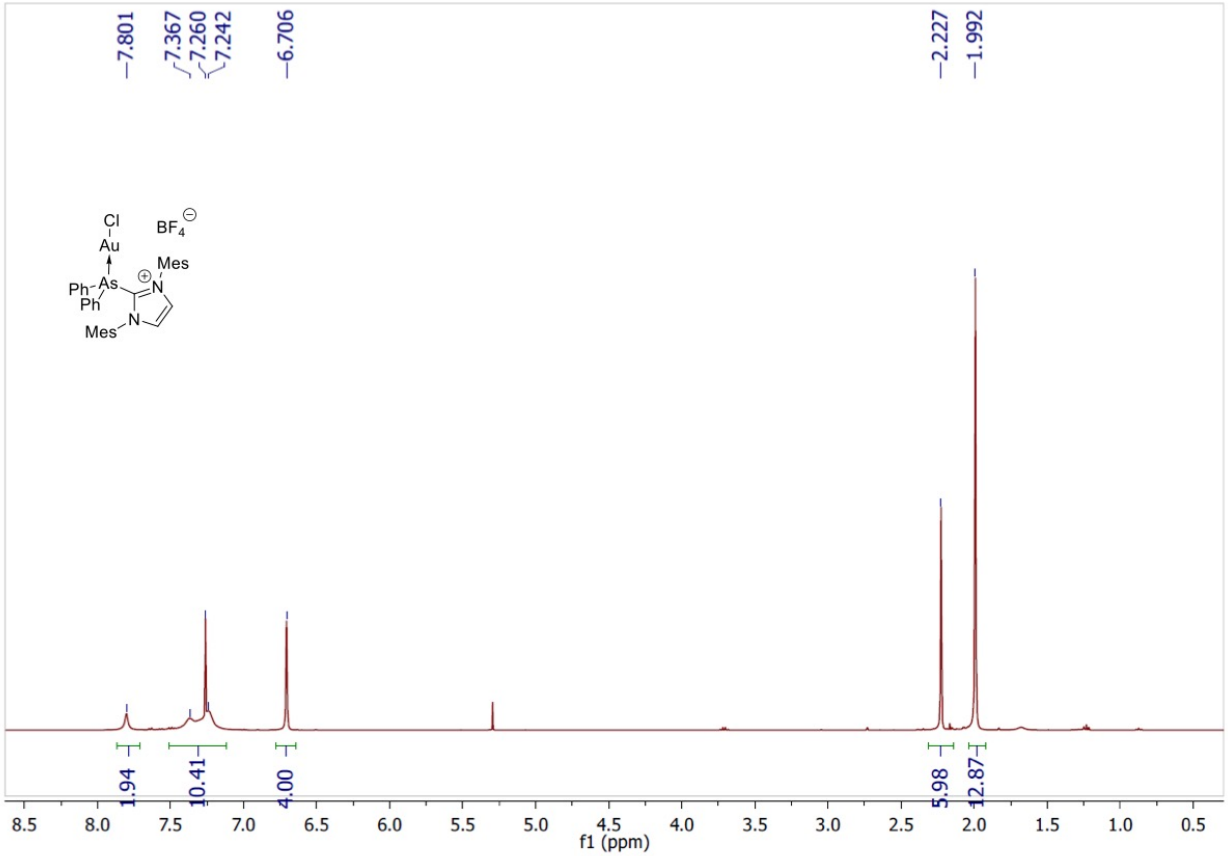
^{1}H-NMR of **17**



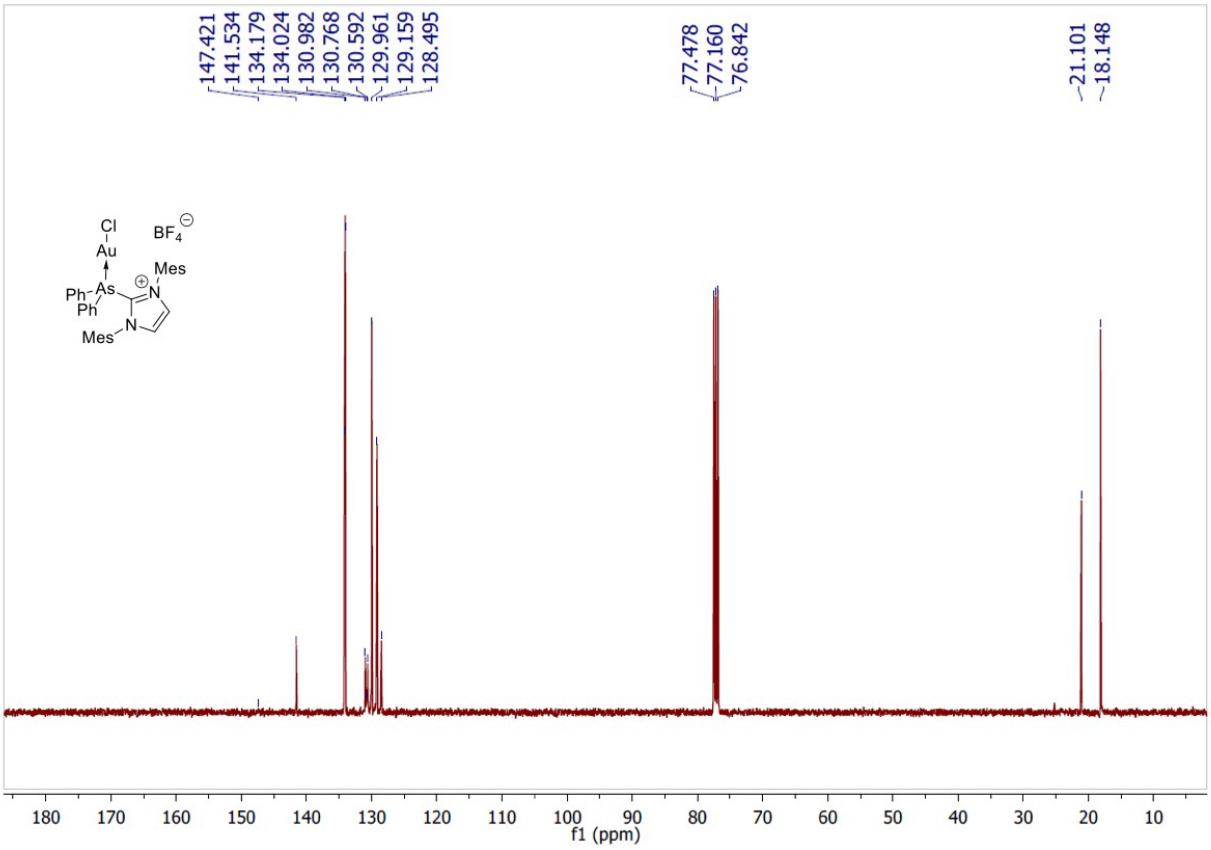
^{13}C-NMR of **17**



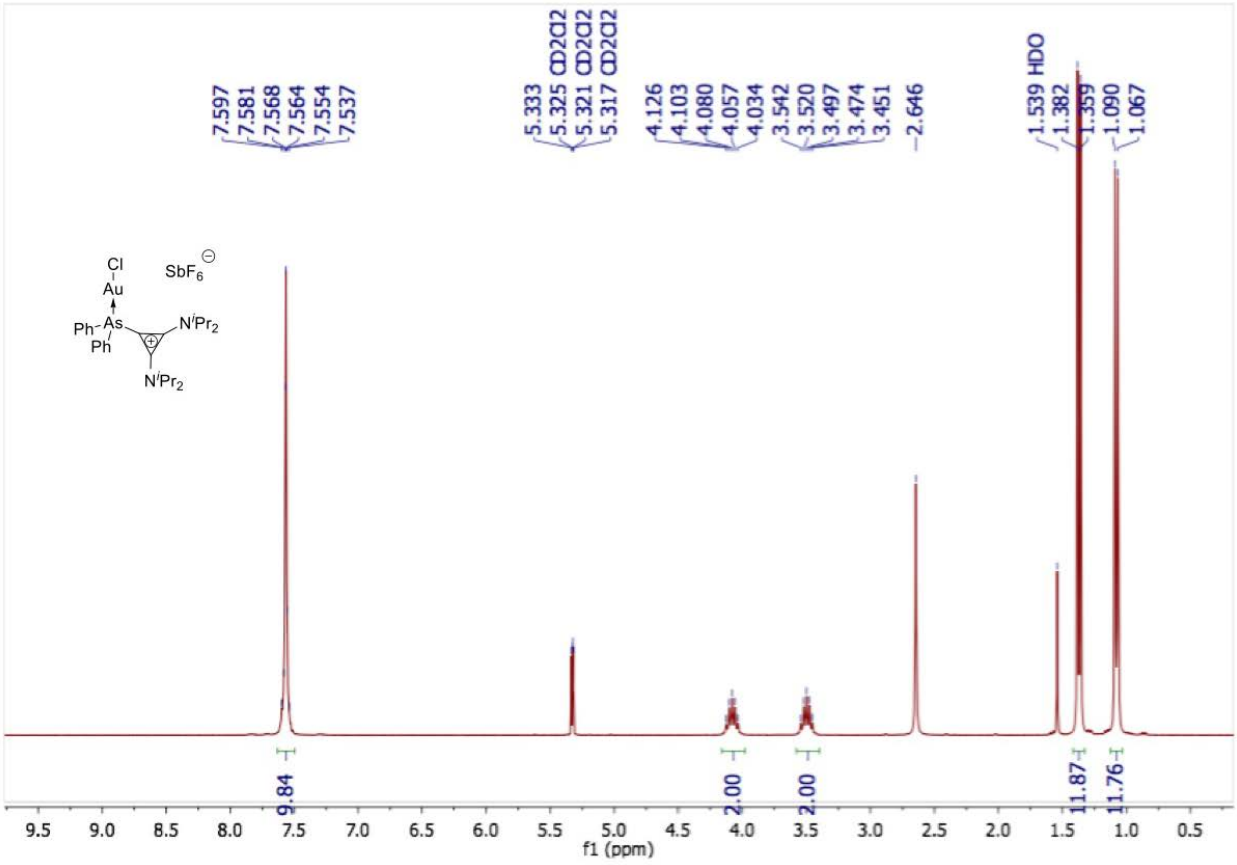
^{1}H-NMR of **19**



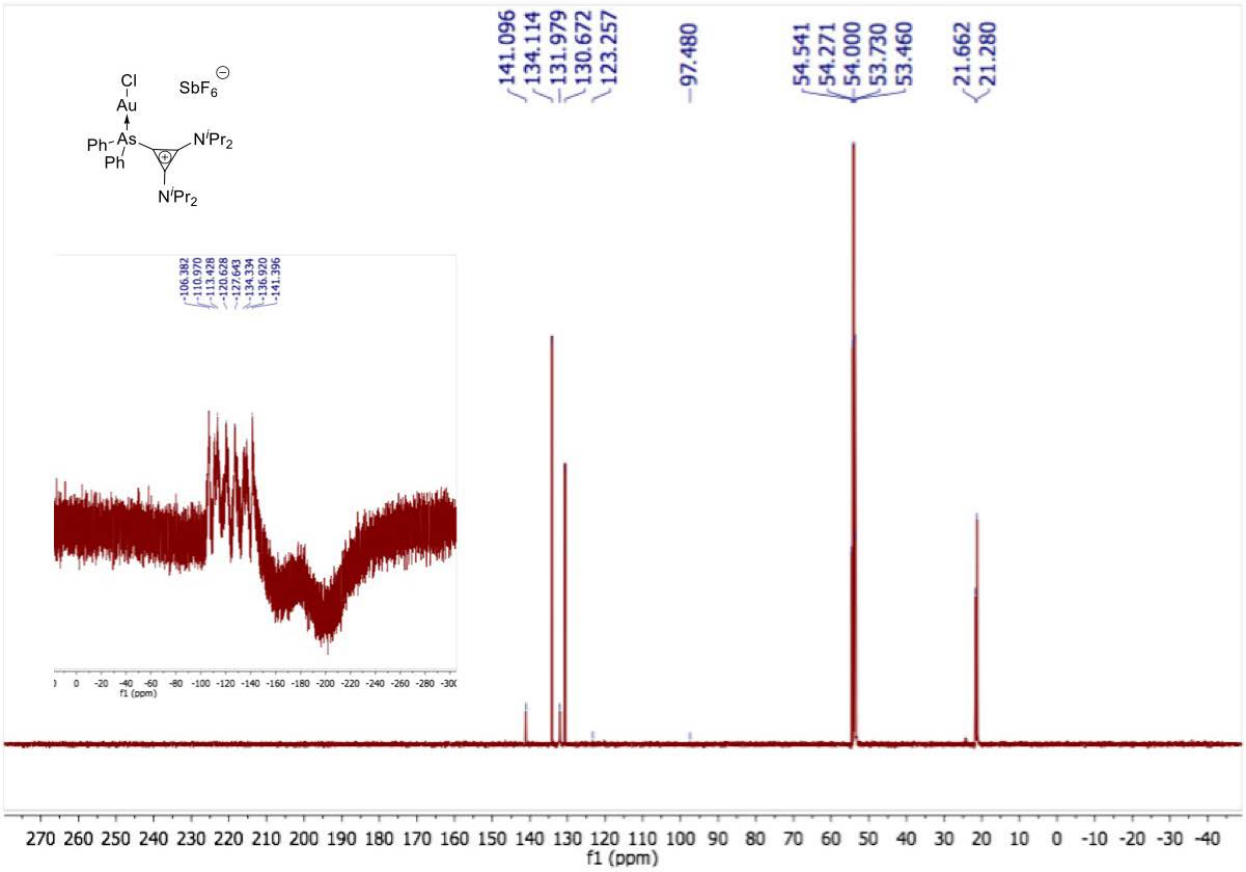
^{13}C-NMR of **19**



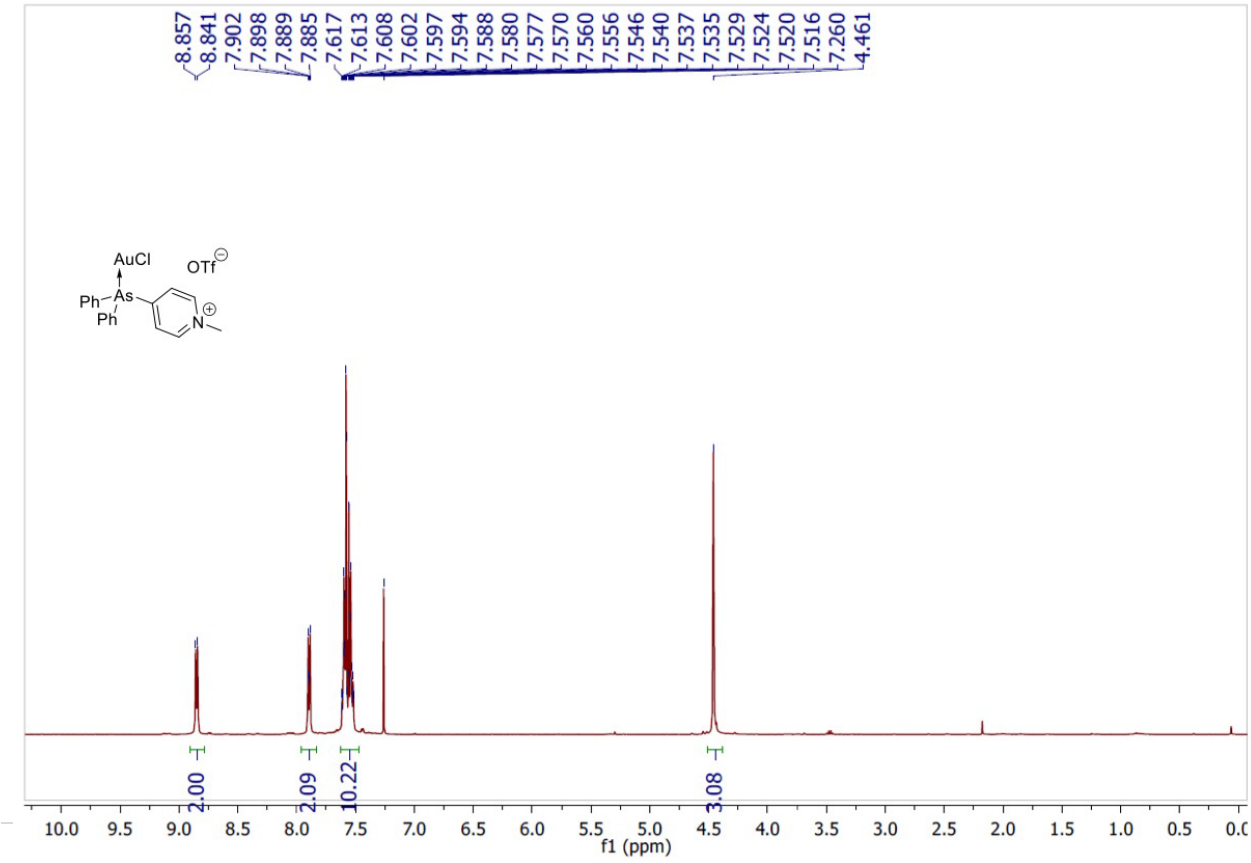
^{1}H-NMR of **21**



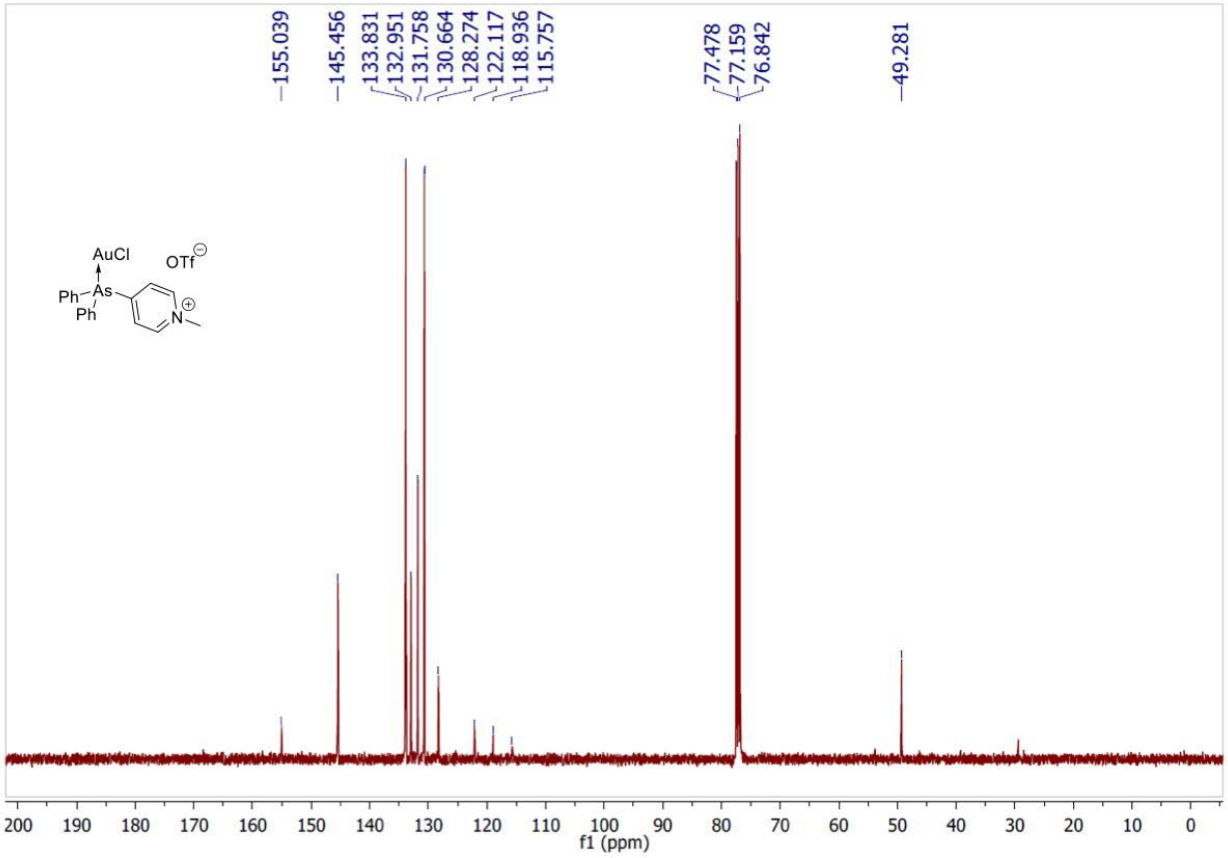
^{13}C-NMR and ^{19}F-NMR (expansion) of **21**



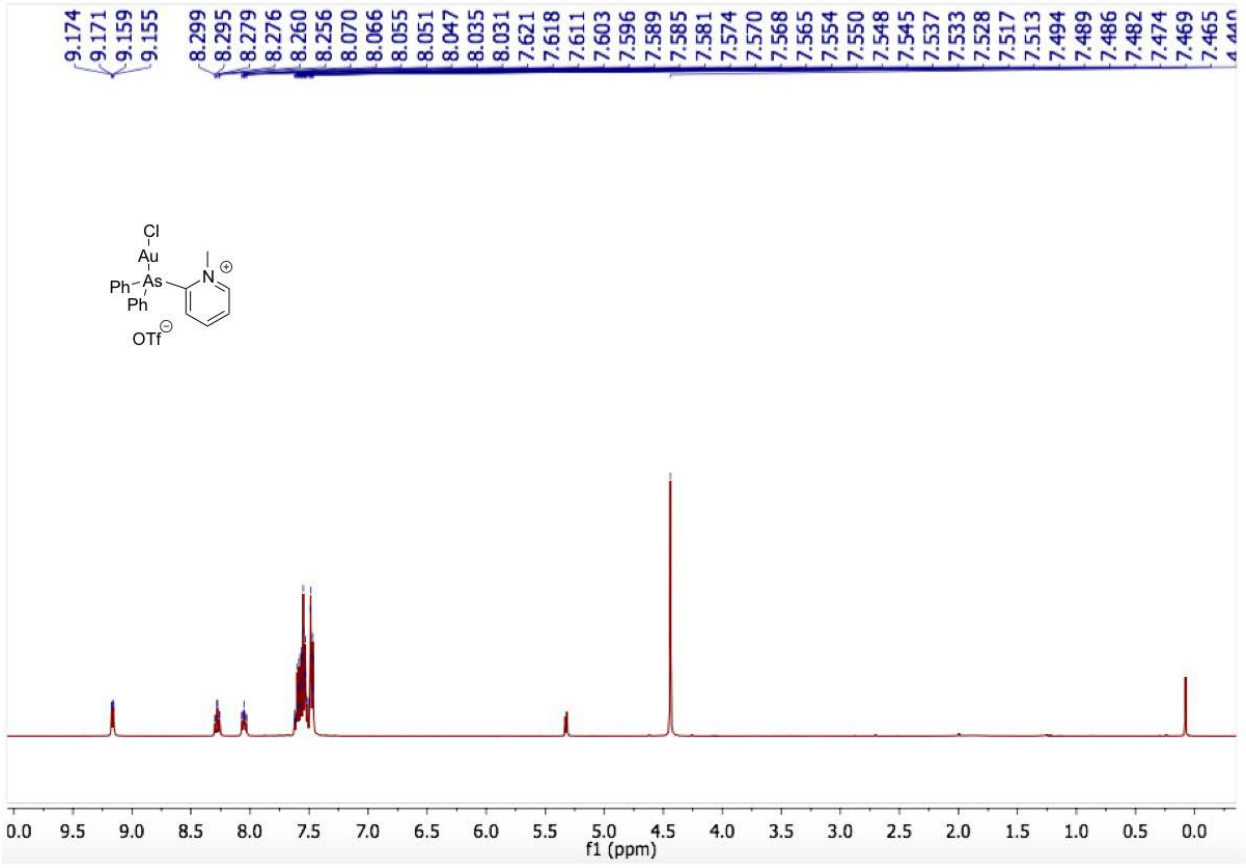
^{1}H-NMR of **22**



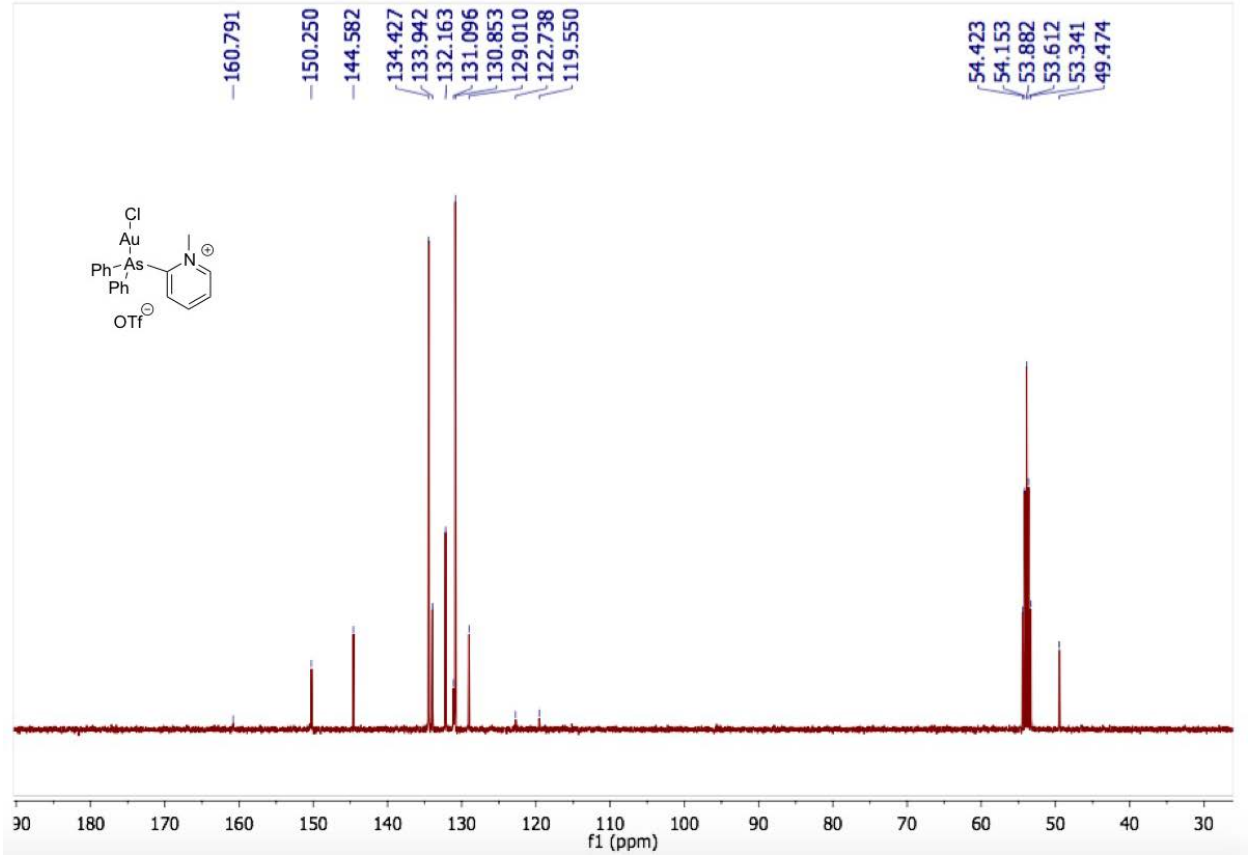
^{13}C-NMR of **22**



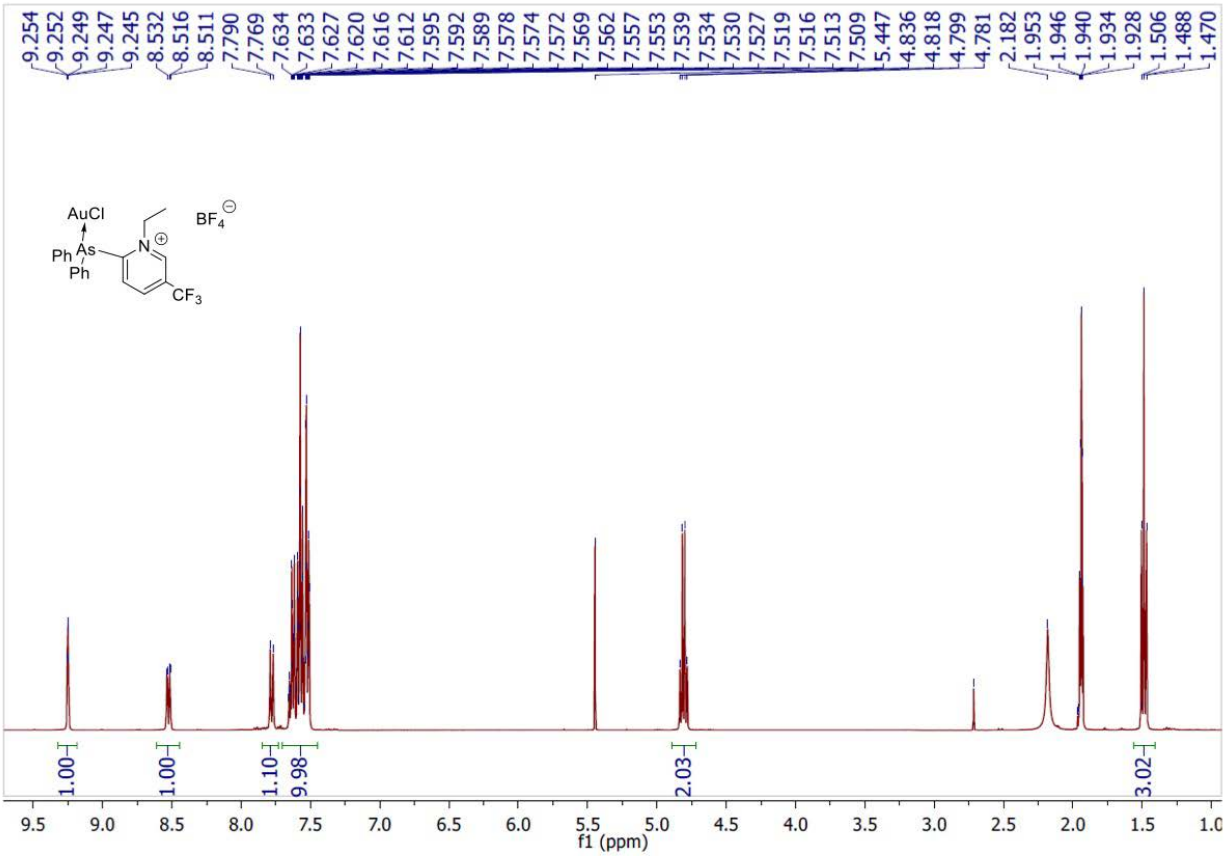
^{1}H-NMR of **23**



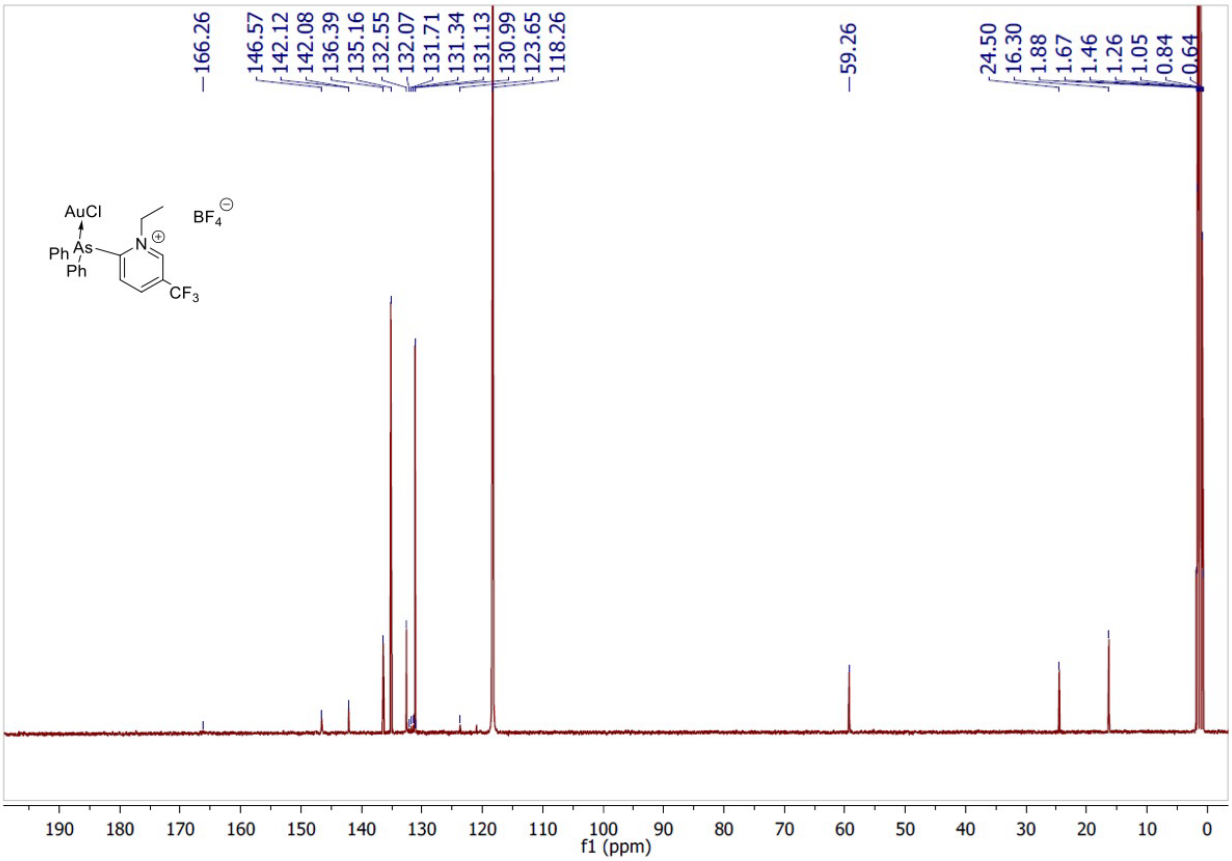
^{13}C-NMR of **23**



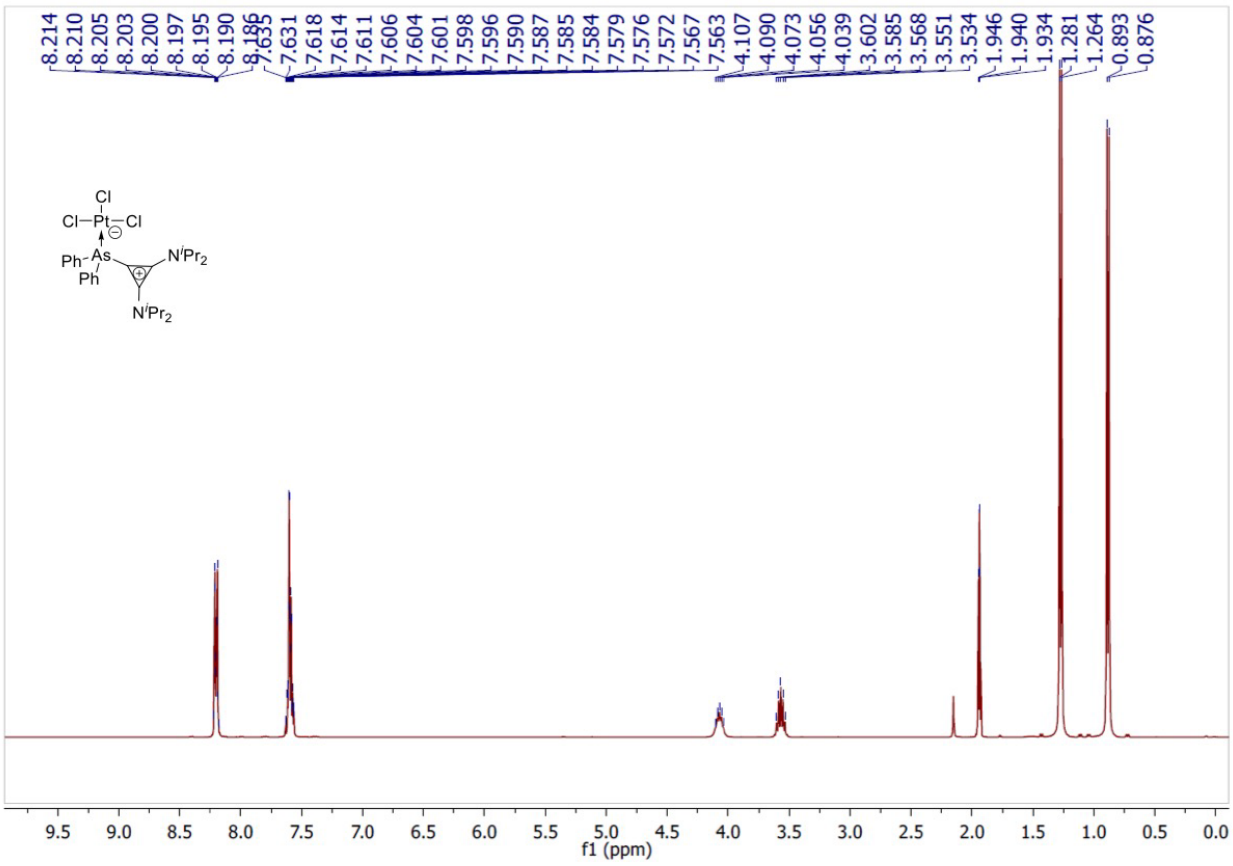
^{1}H-NMR of **24**



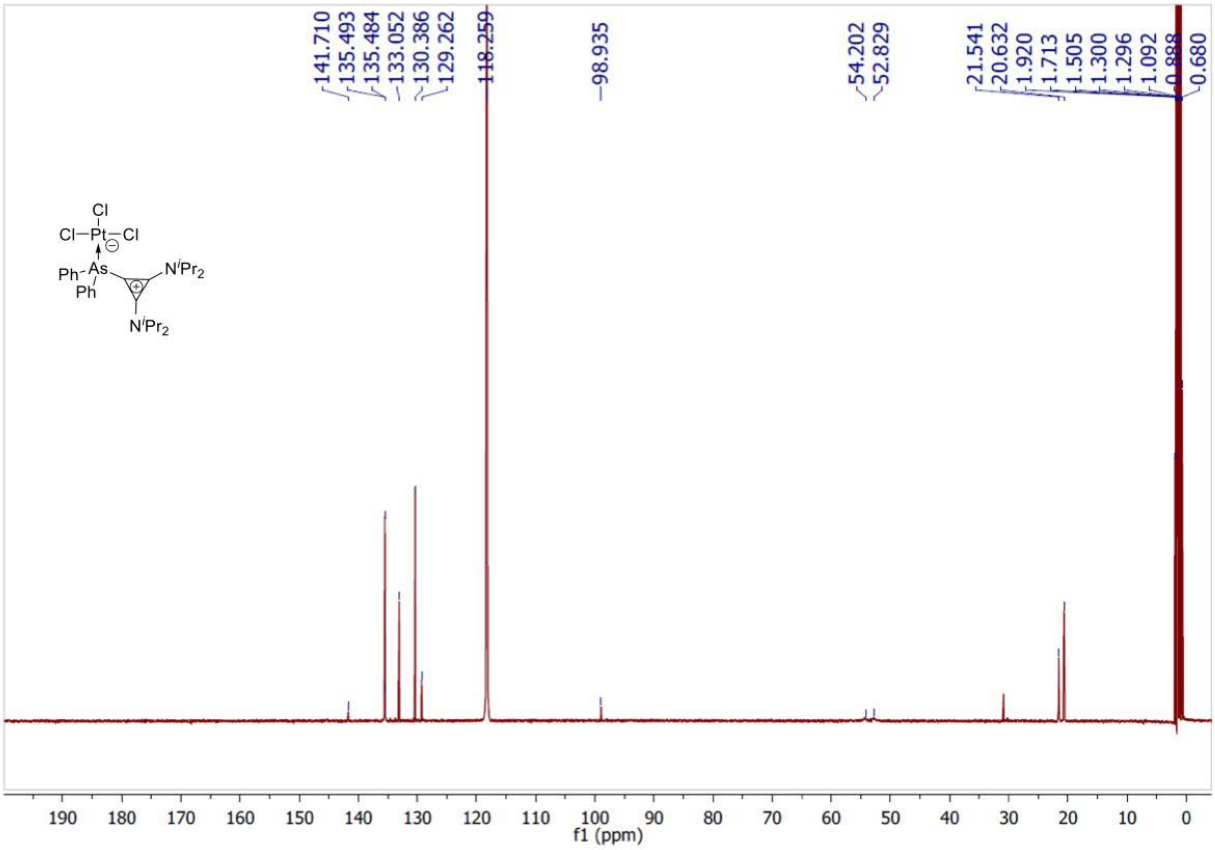
^{13}C-NMR of **24**



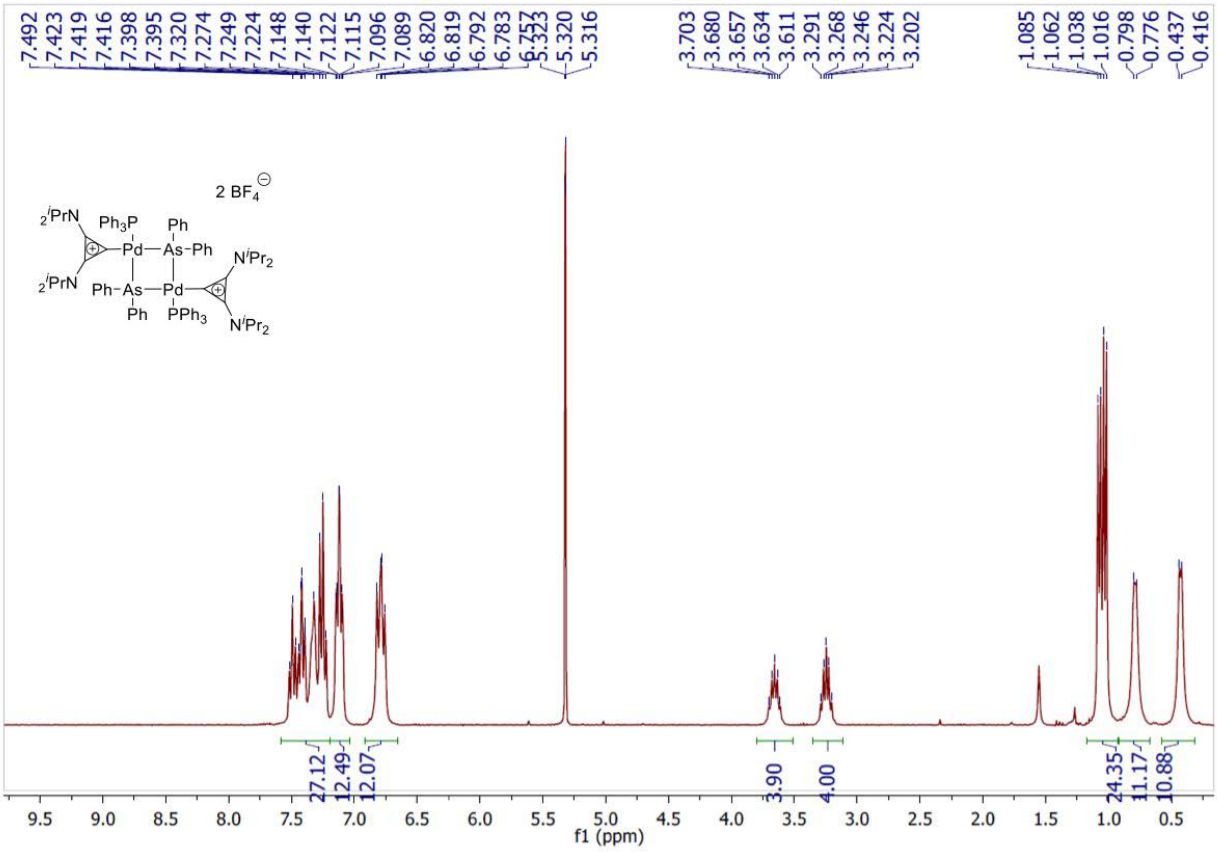
^{1}H-NMR of **25**



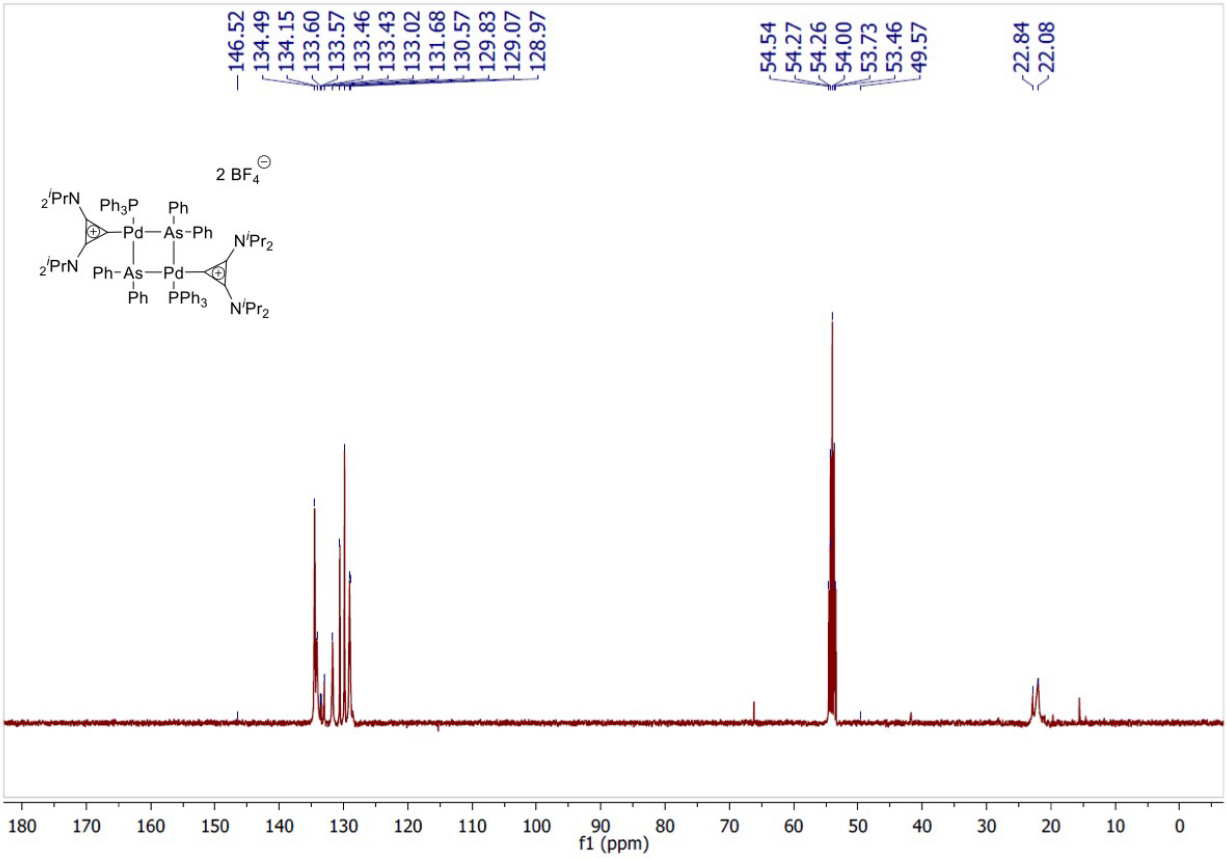
^{13}C-NMR of **25**



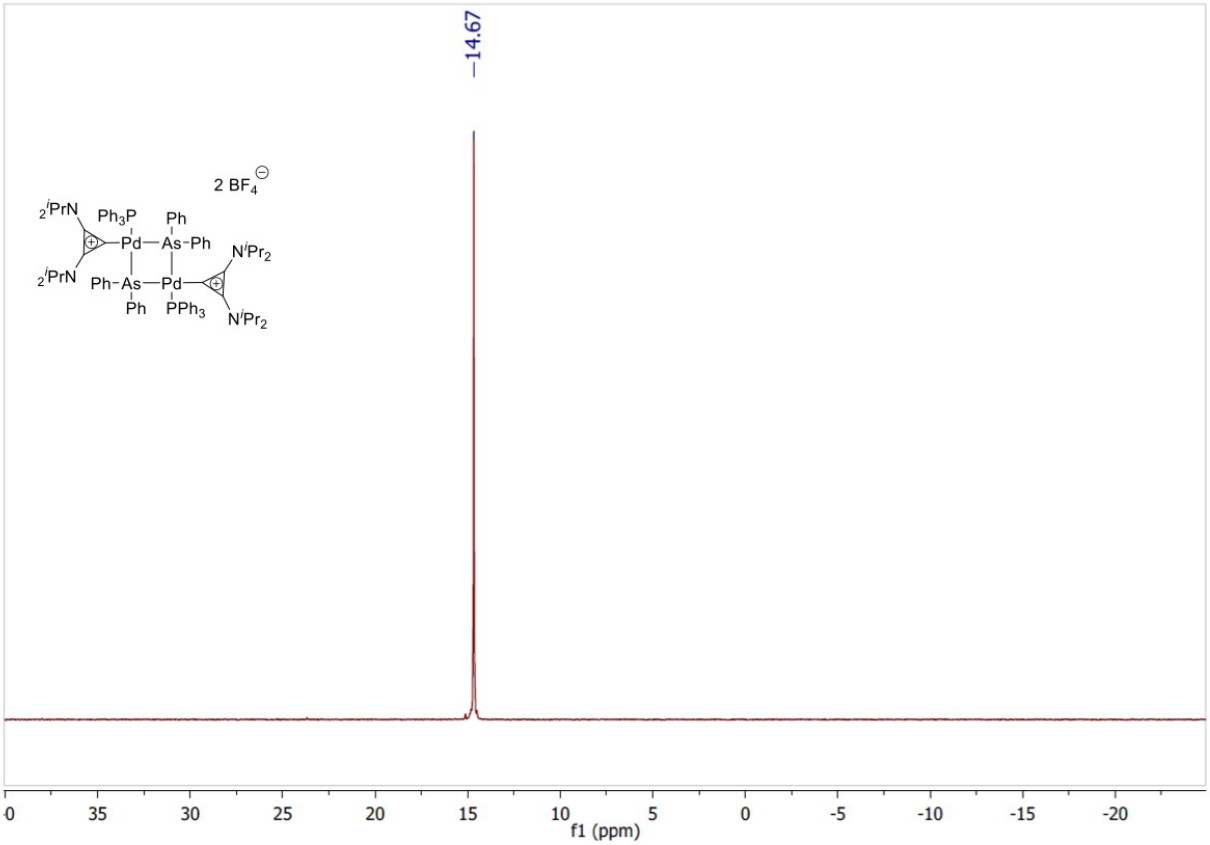
^{1}H-NMR of **27**



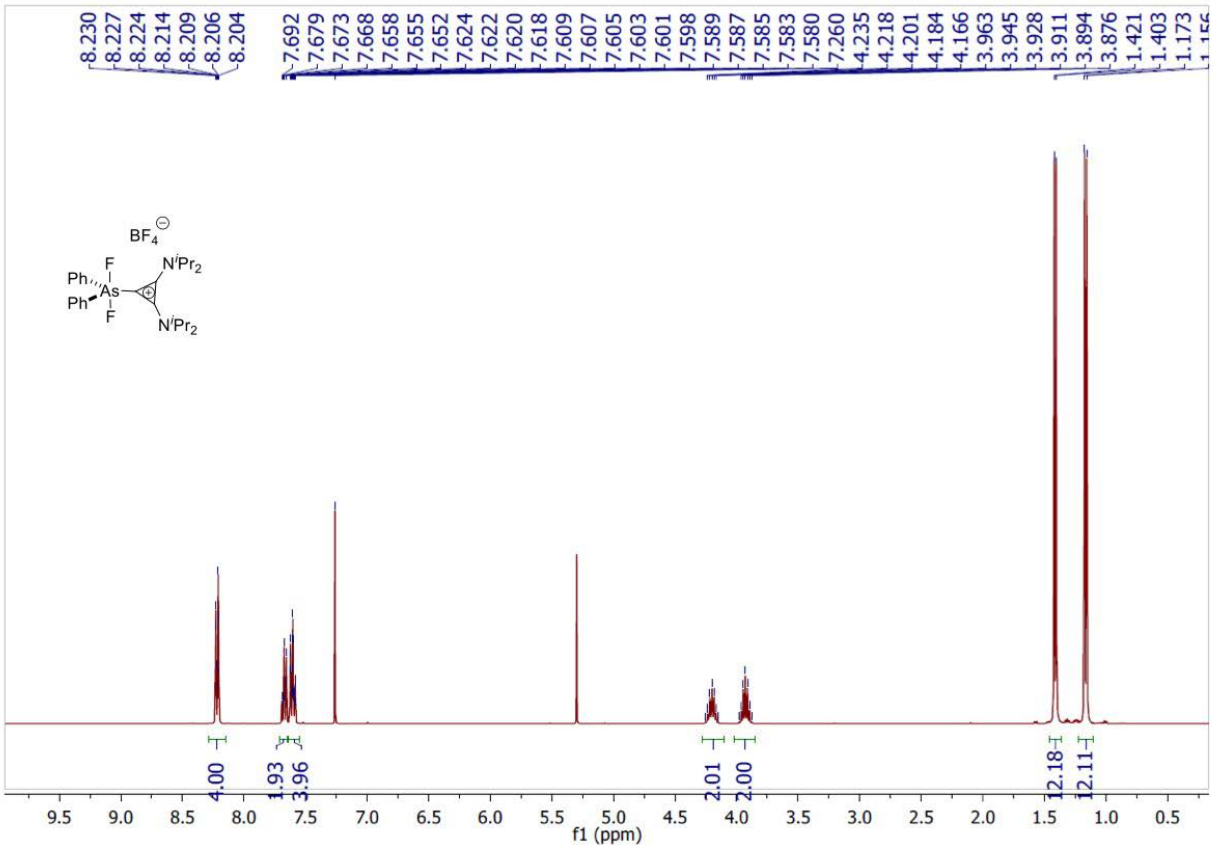
^{13}C-NMR of **27**



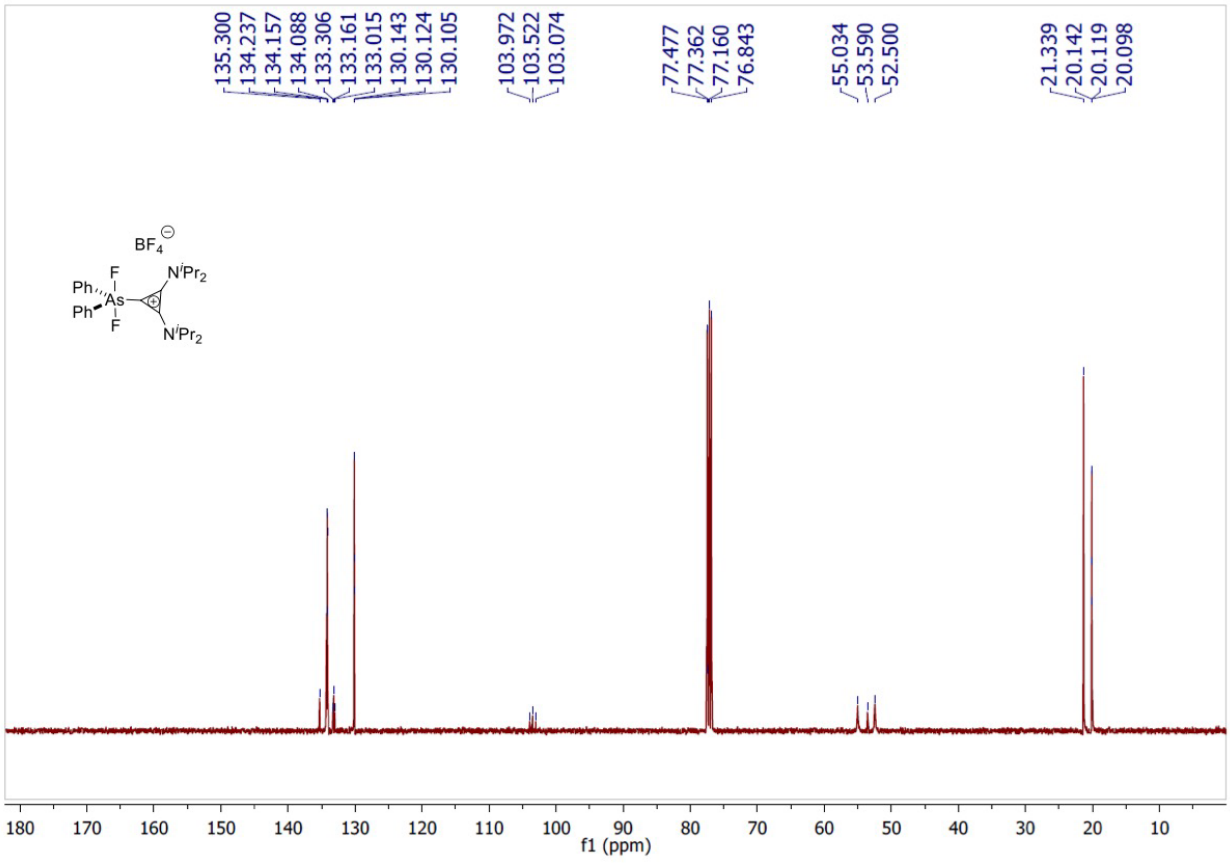
^{31}P-NMR of **27**



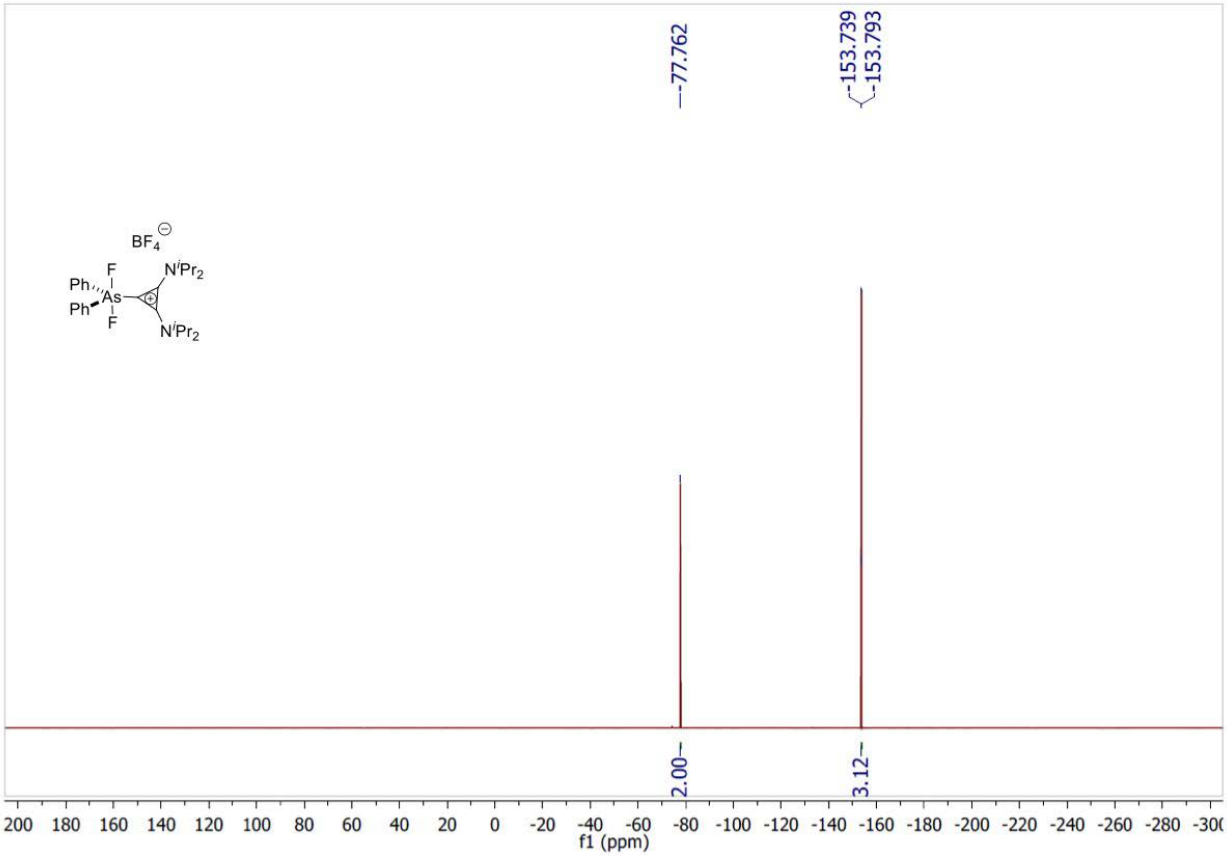
^{1}H-NMR of **28**



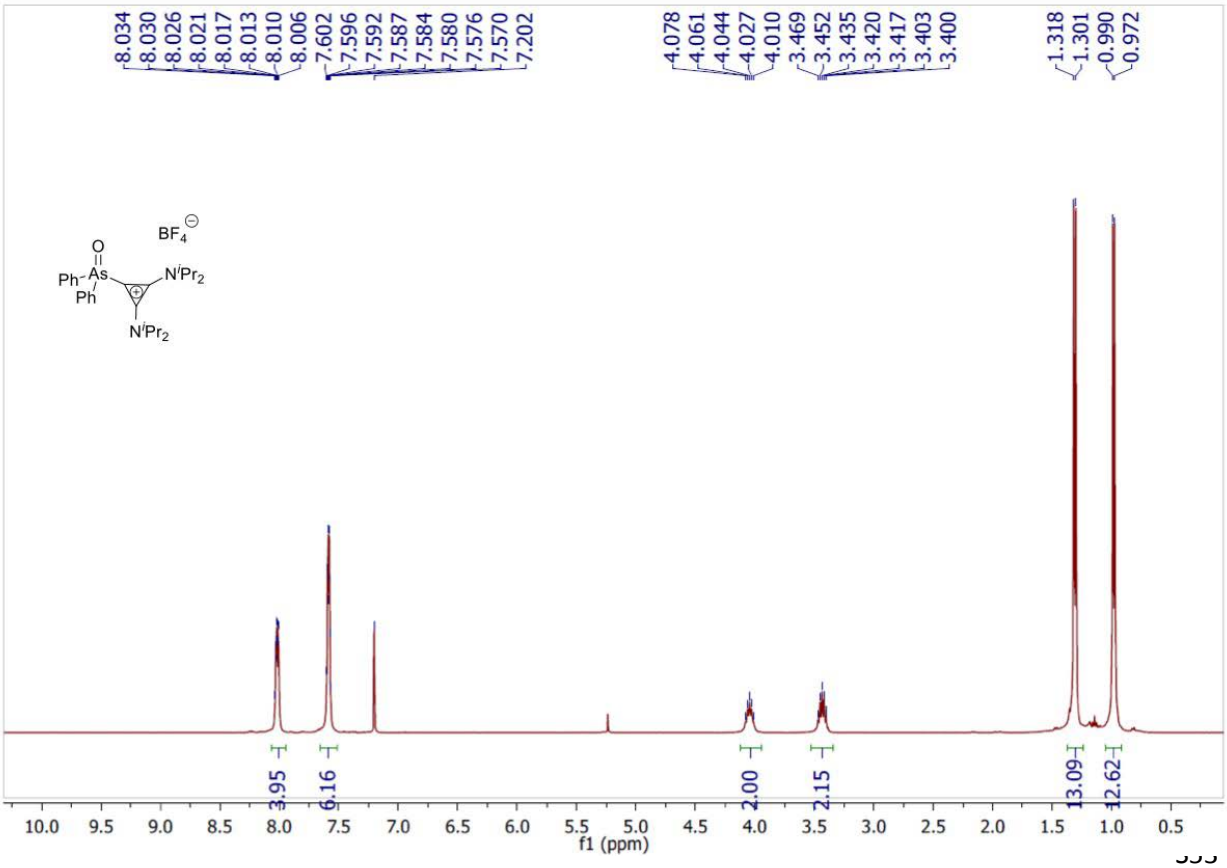
^{13}C-NMR of **28**



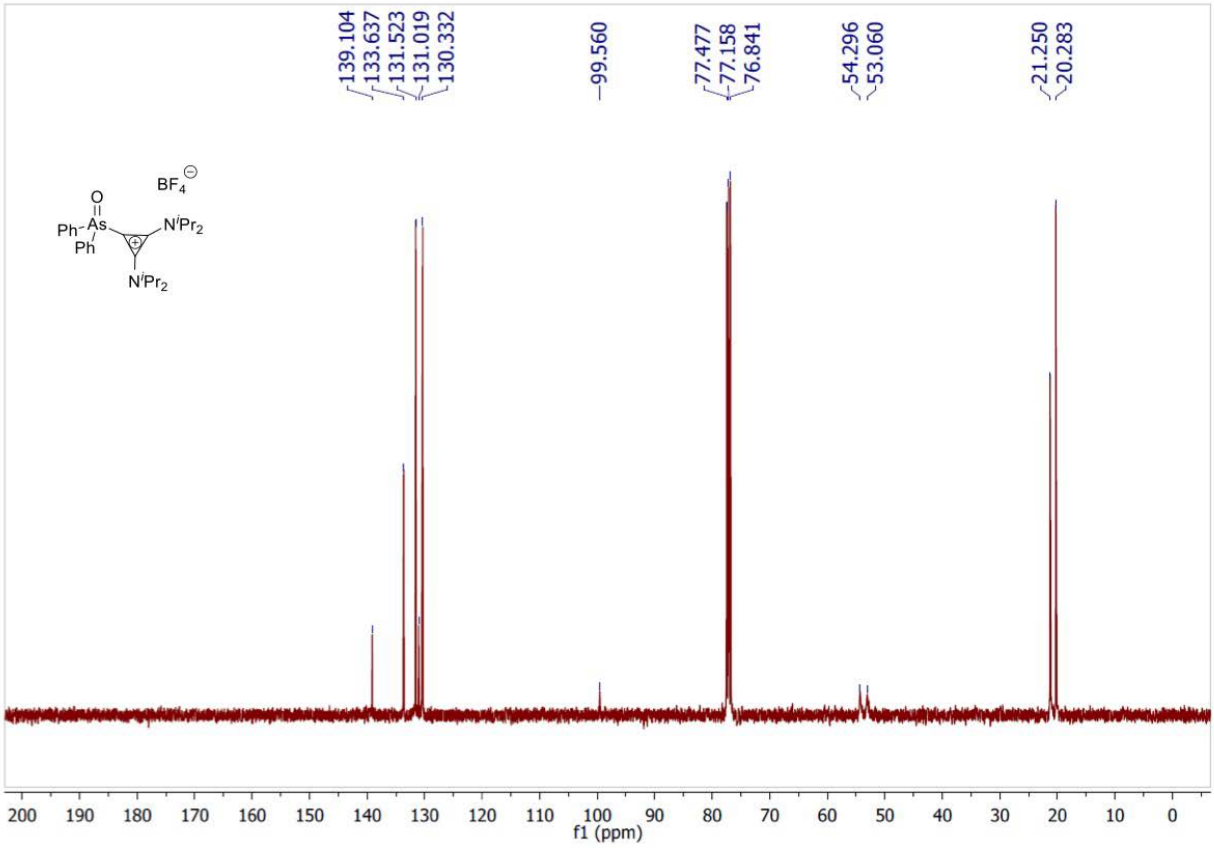
^{19}F-NMR of **28**



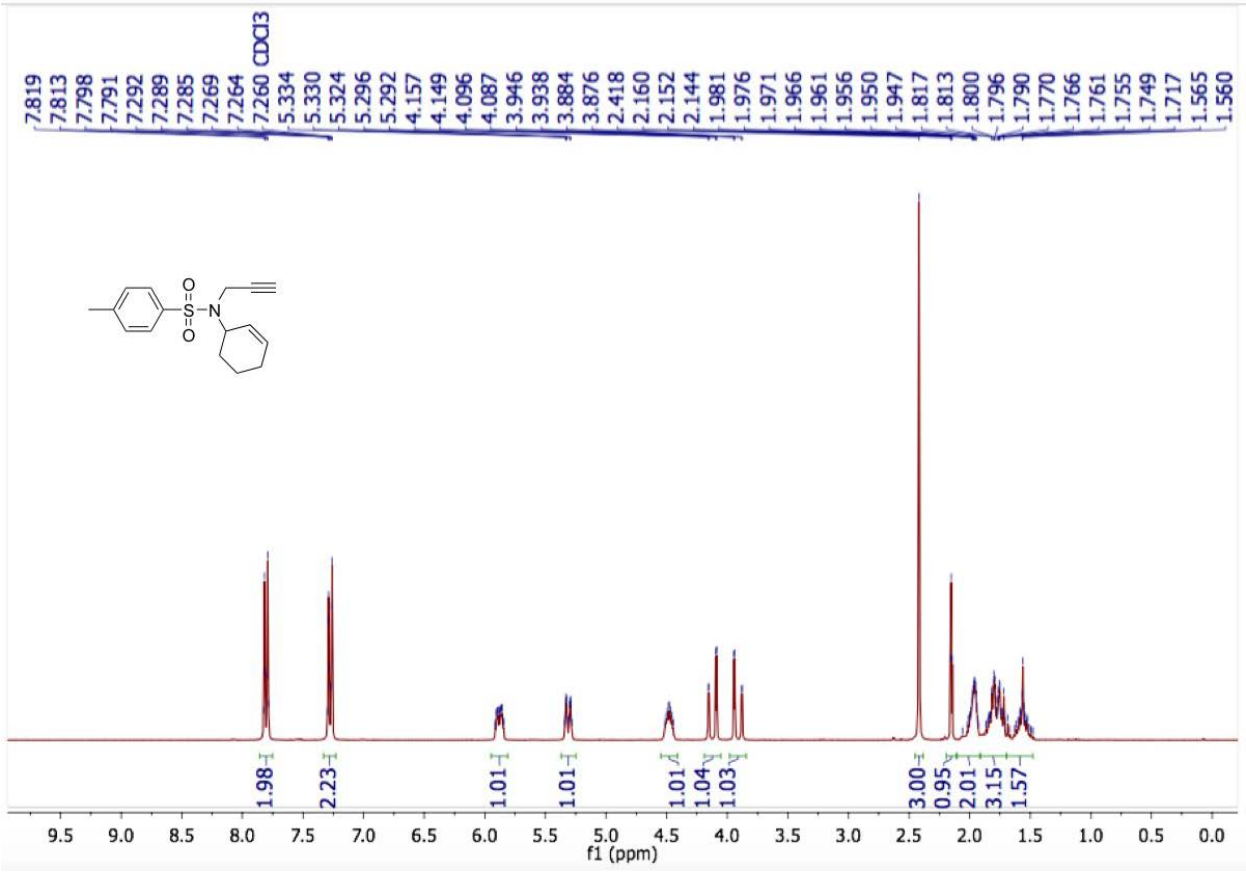
^{1}H-NMR of **29**



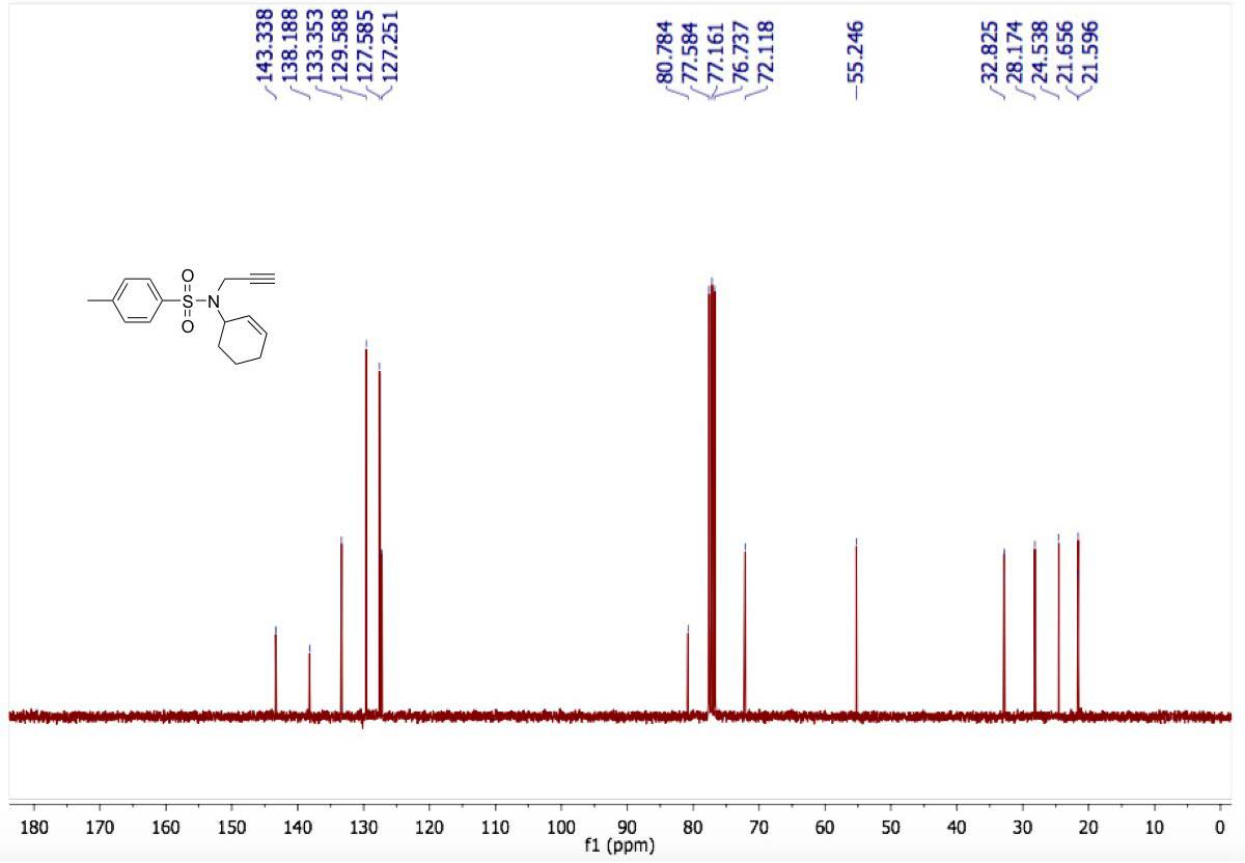
^{13}C-NMR of **29**



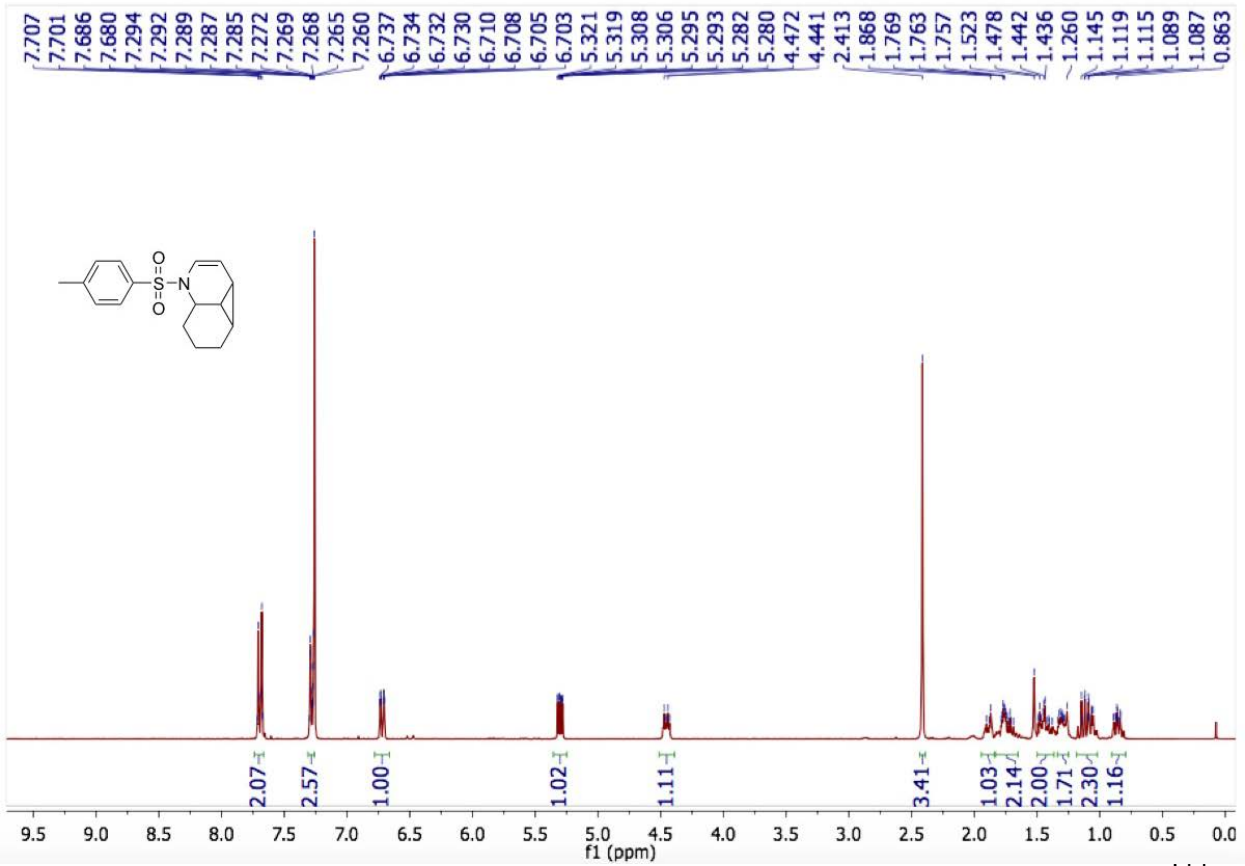
^{1}H-NMR of **30**



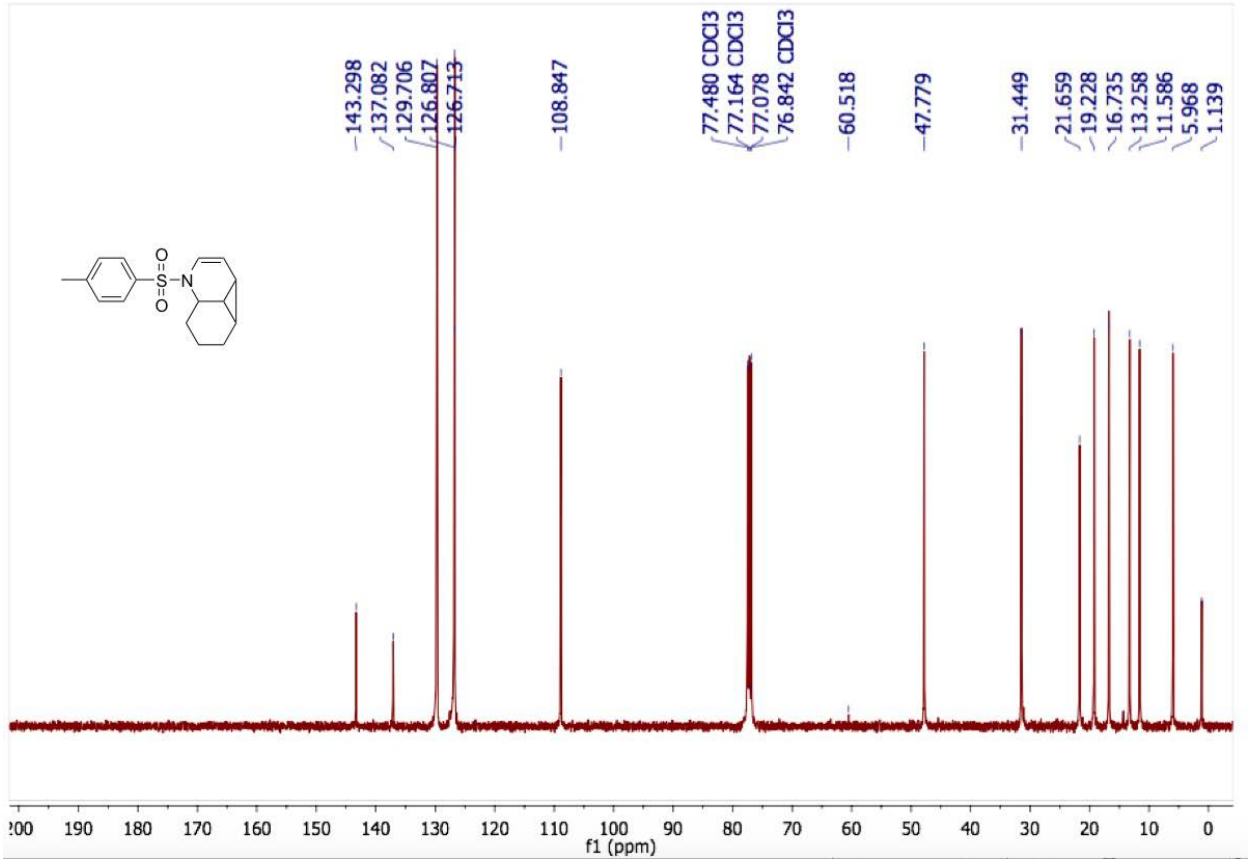
^{13}C-NMR of **30**



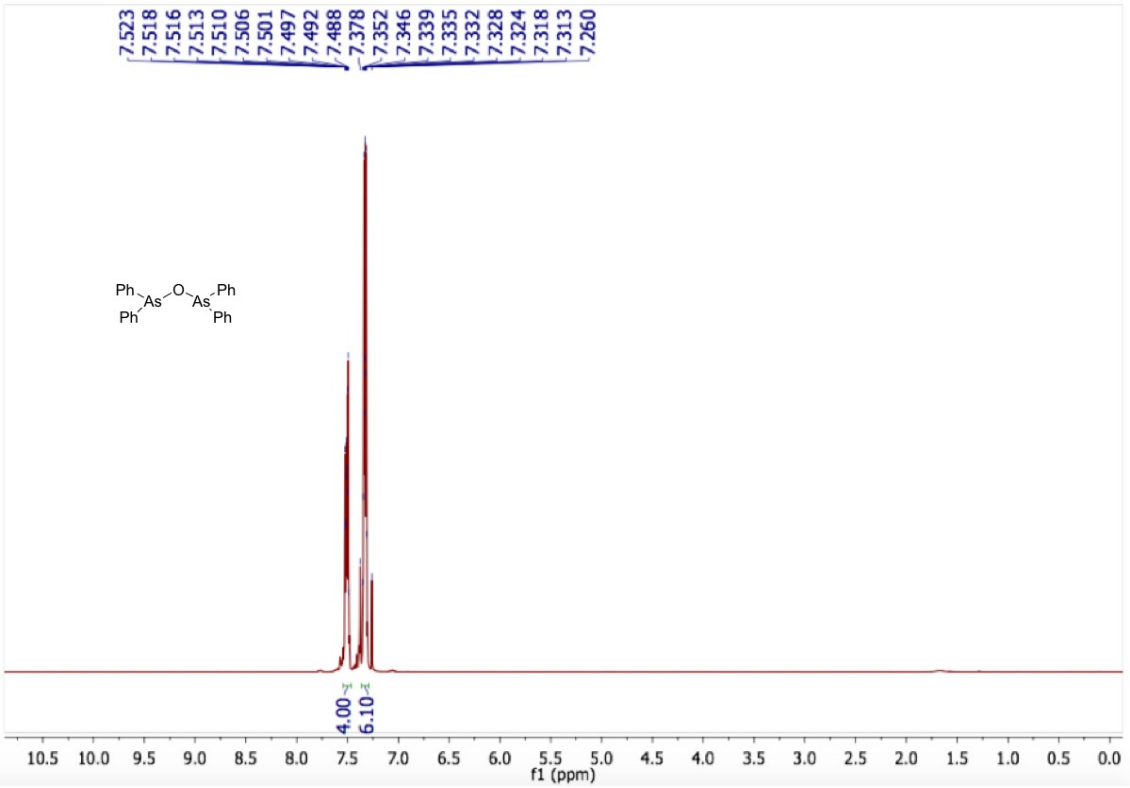
^{1}H-NMR of **31**

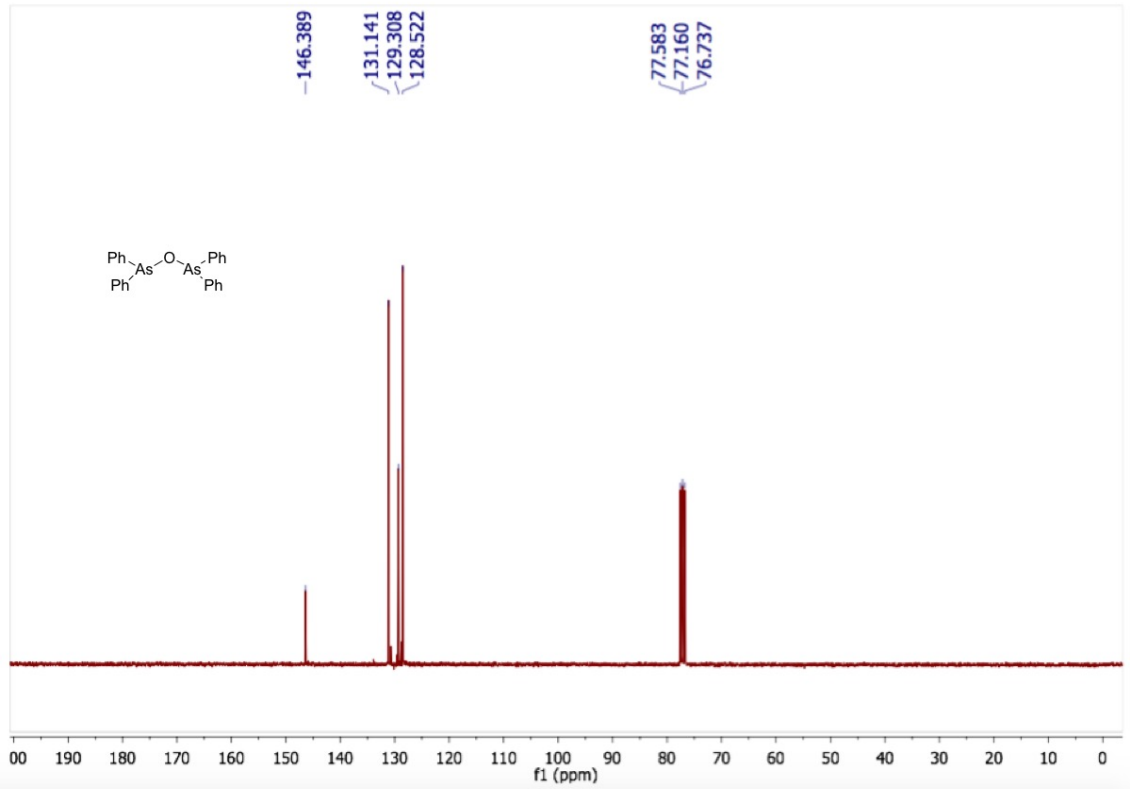


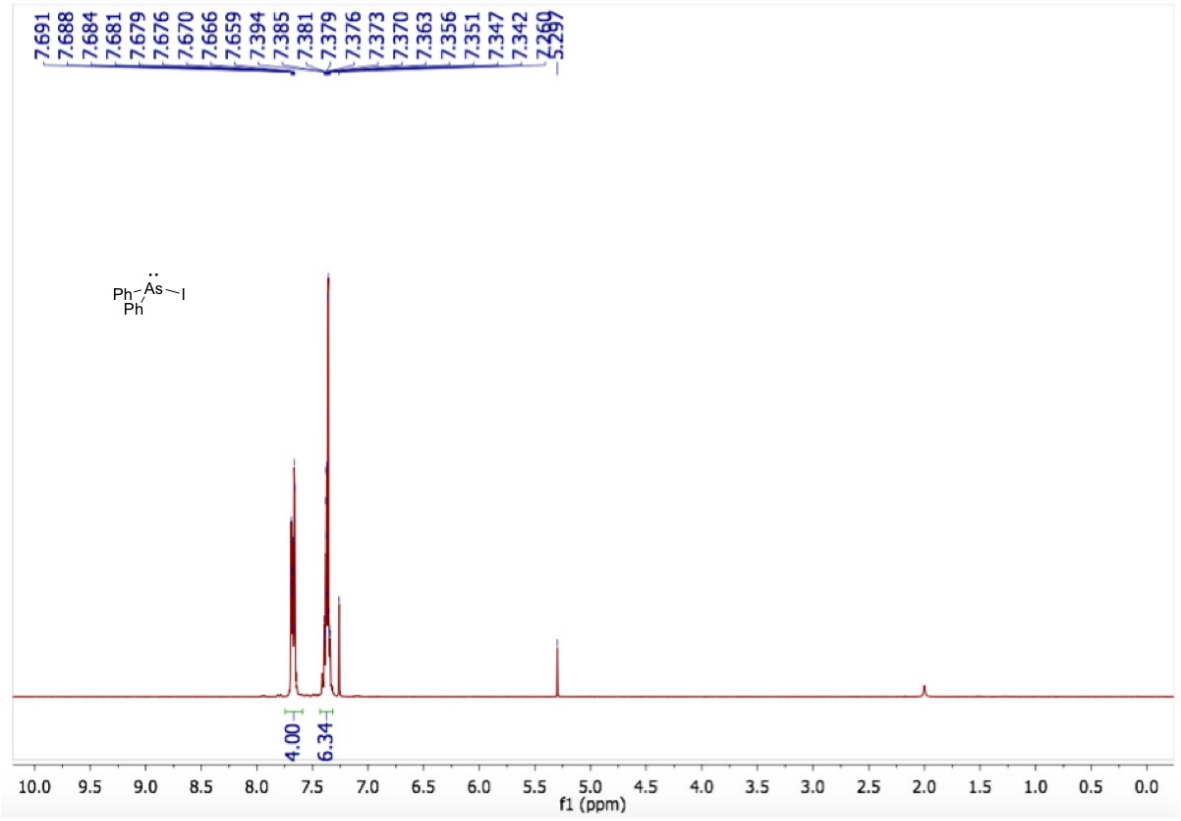
^{13}C-NMR of **31**

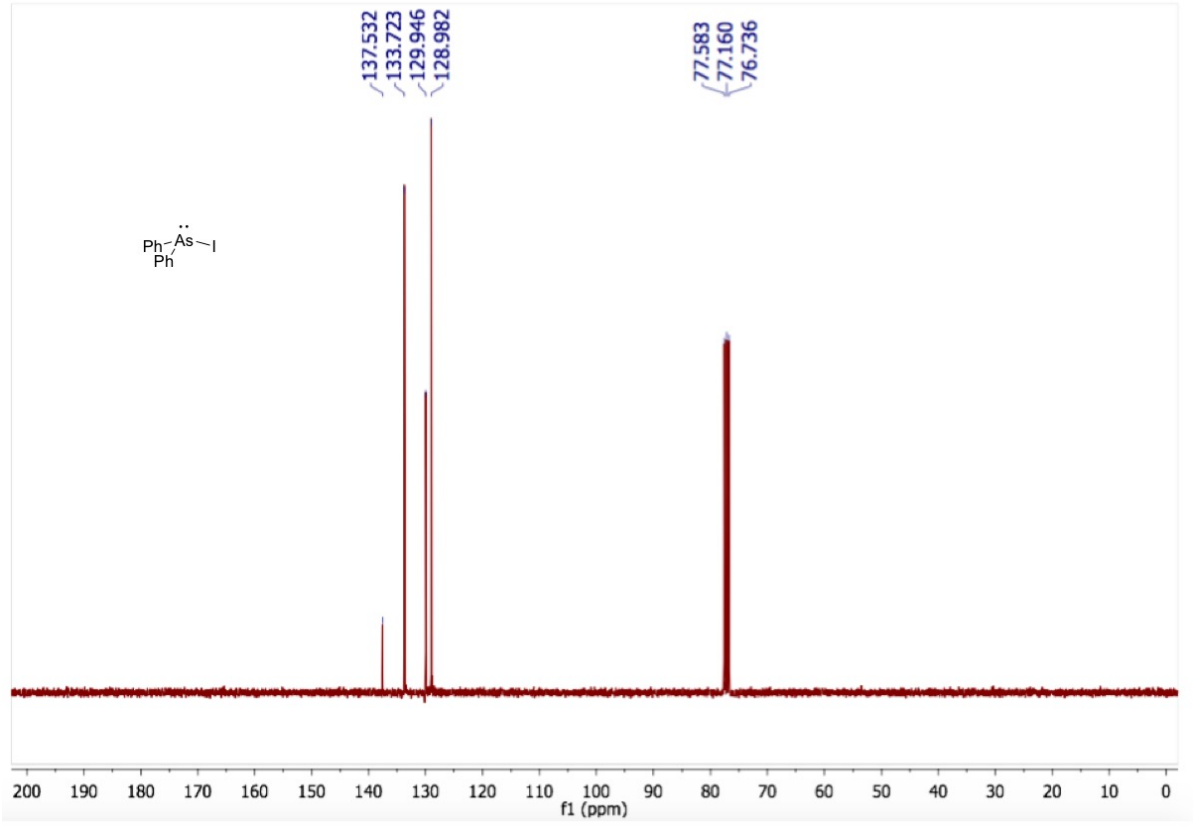

143.298
137.082
129.706
126.807
126.713
108.847
77.480 CDCl3
77.164 CDCl3
77.078
76.842 CDCl3
60.518
47.779
31.449
21.659
19.228
16.735
13.258
11.586
5.968
1.139
O
S
N
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

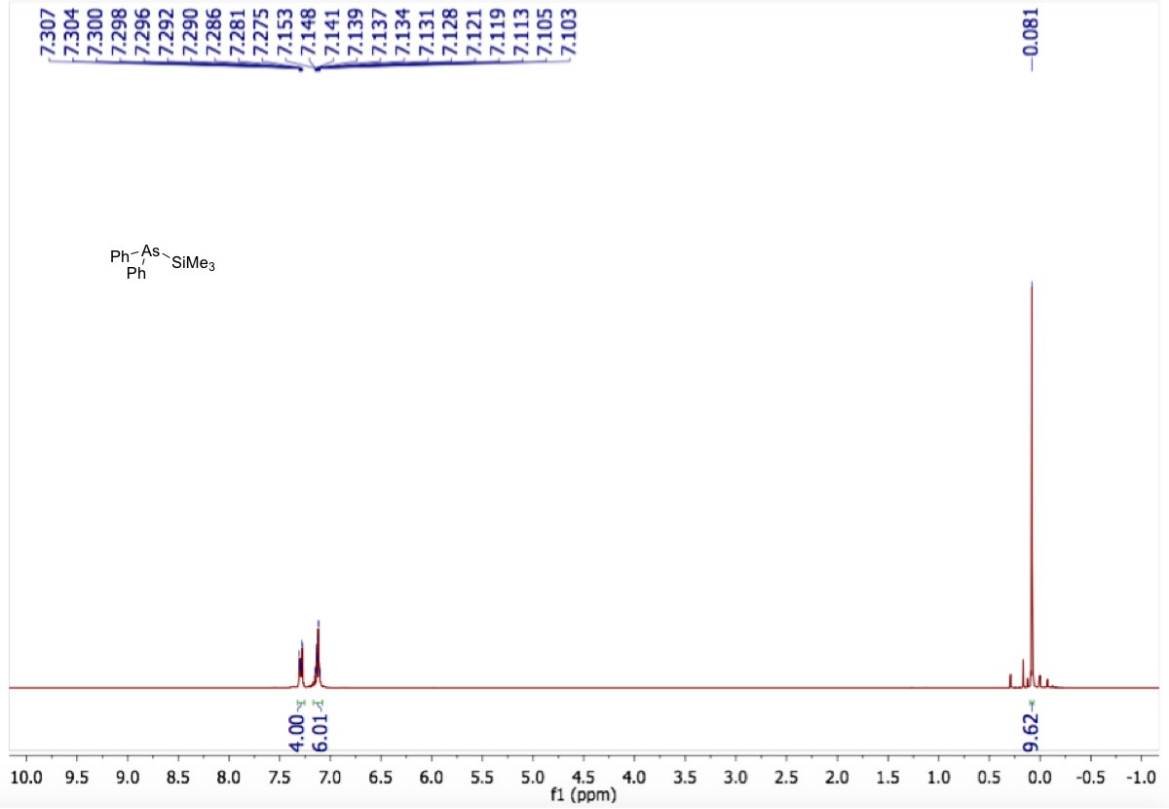
NMR Spectra for Starting Reagents:

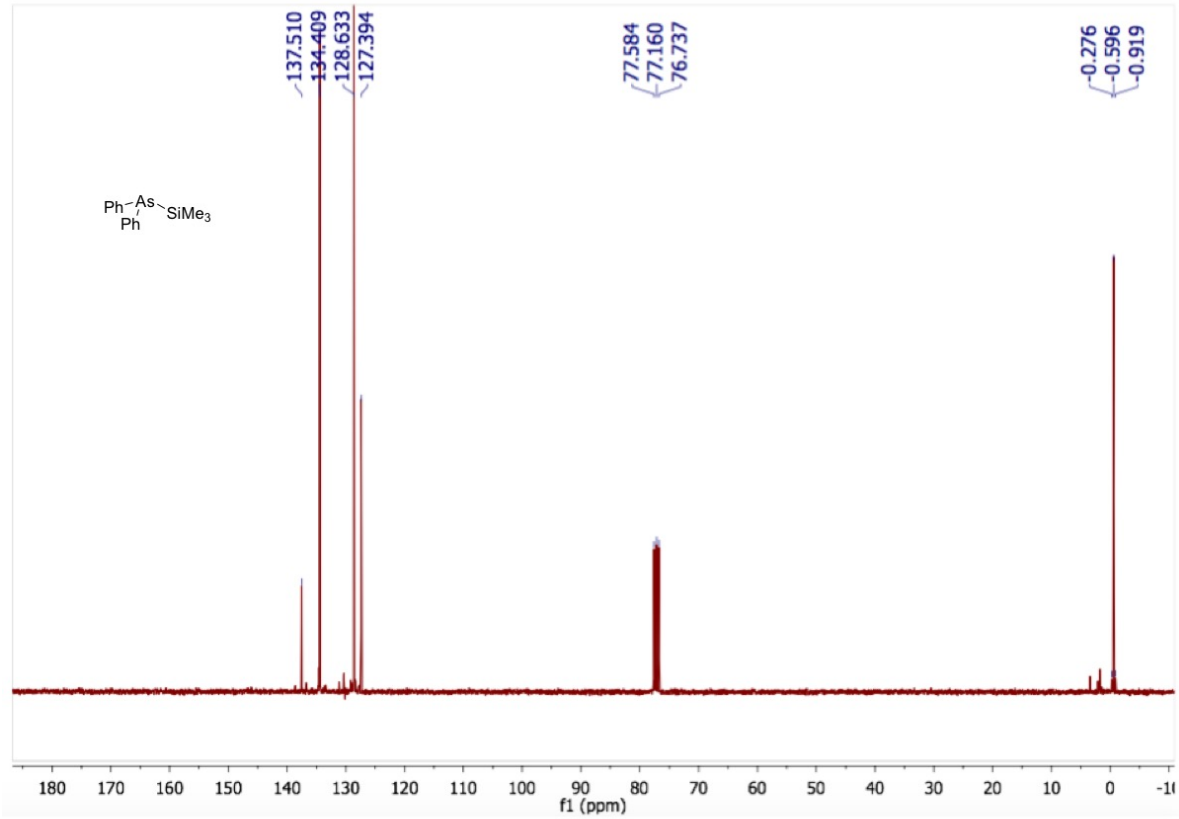


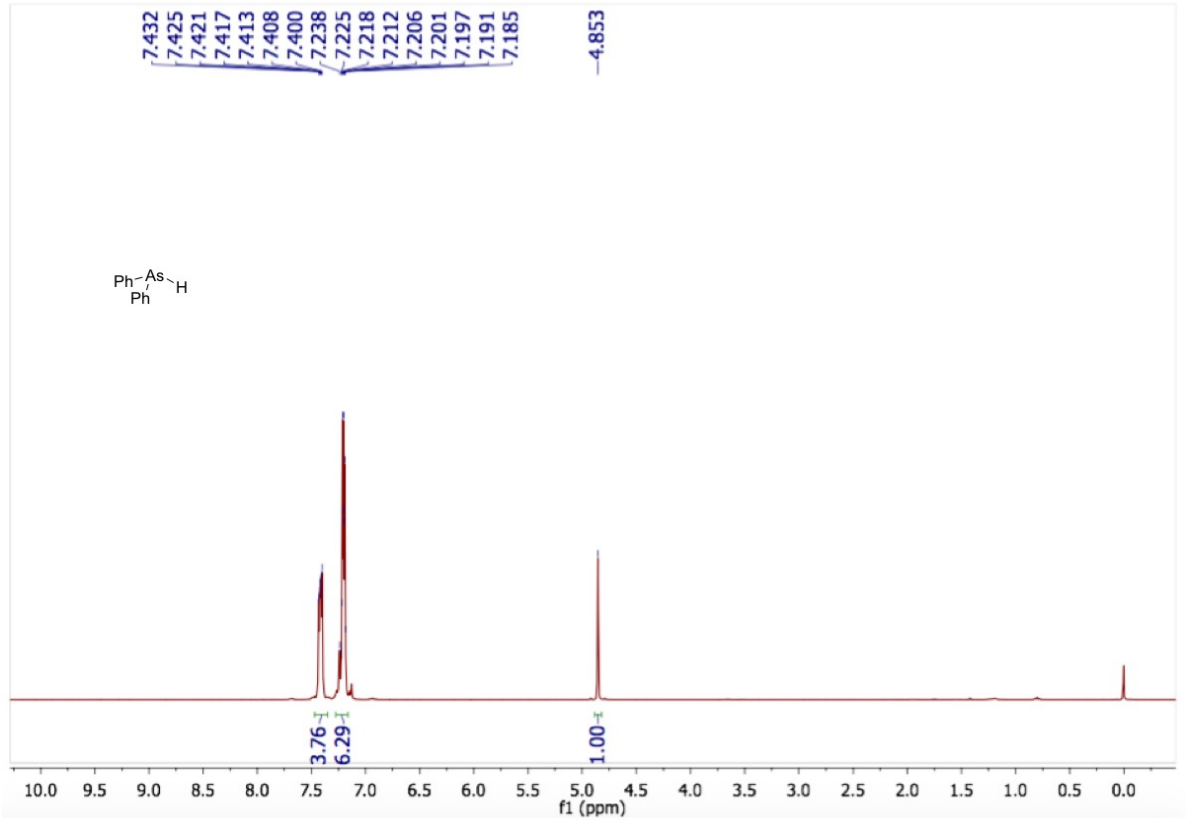


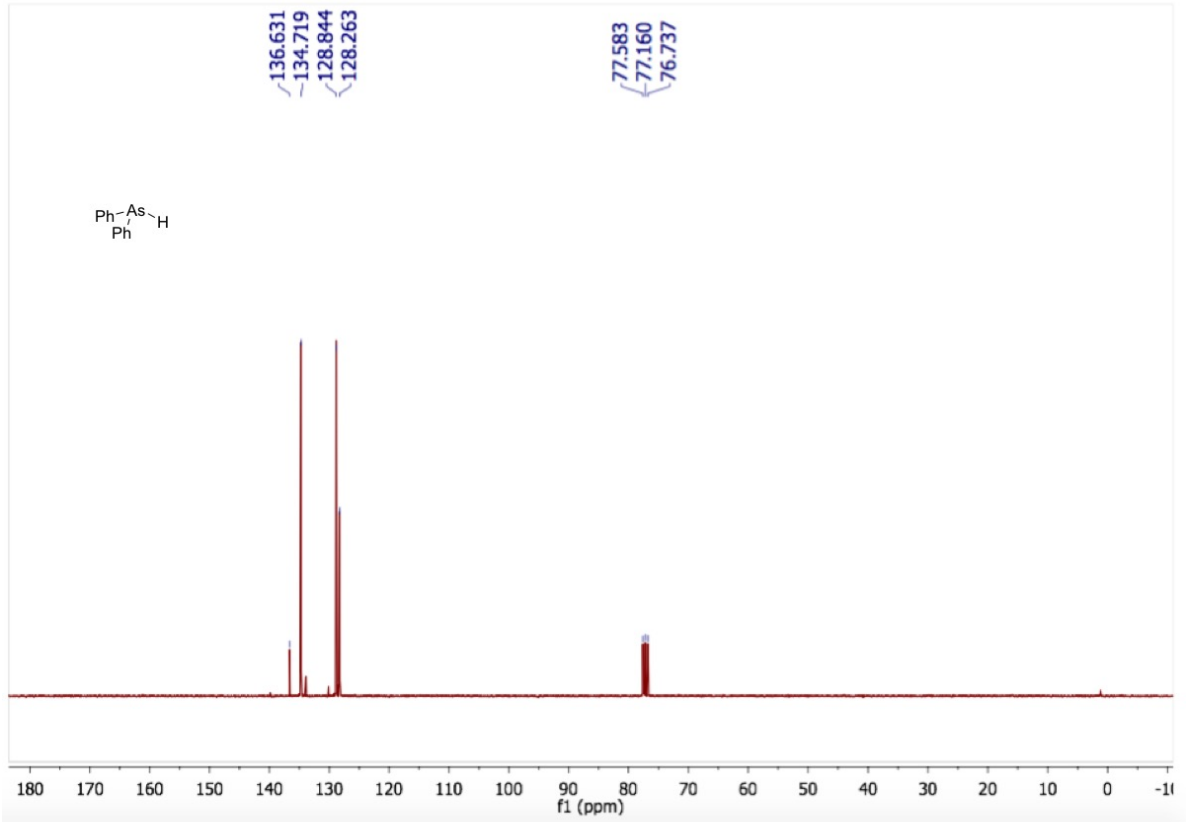

7.691
7.688
7.684
7.681
7.679
7.676
7.670
7.666
7.659
7.394
7.385
7.381
7.379
7.376
7.373
7.370
7.363
7.356
7.351
7.347
7.342
5.297
Ph
As
I
Ph
4.00
6.34
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

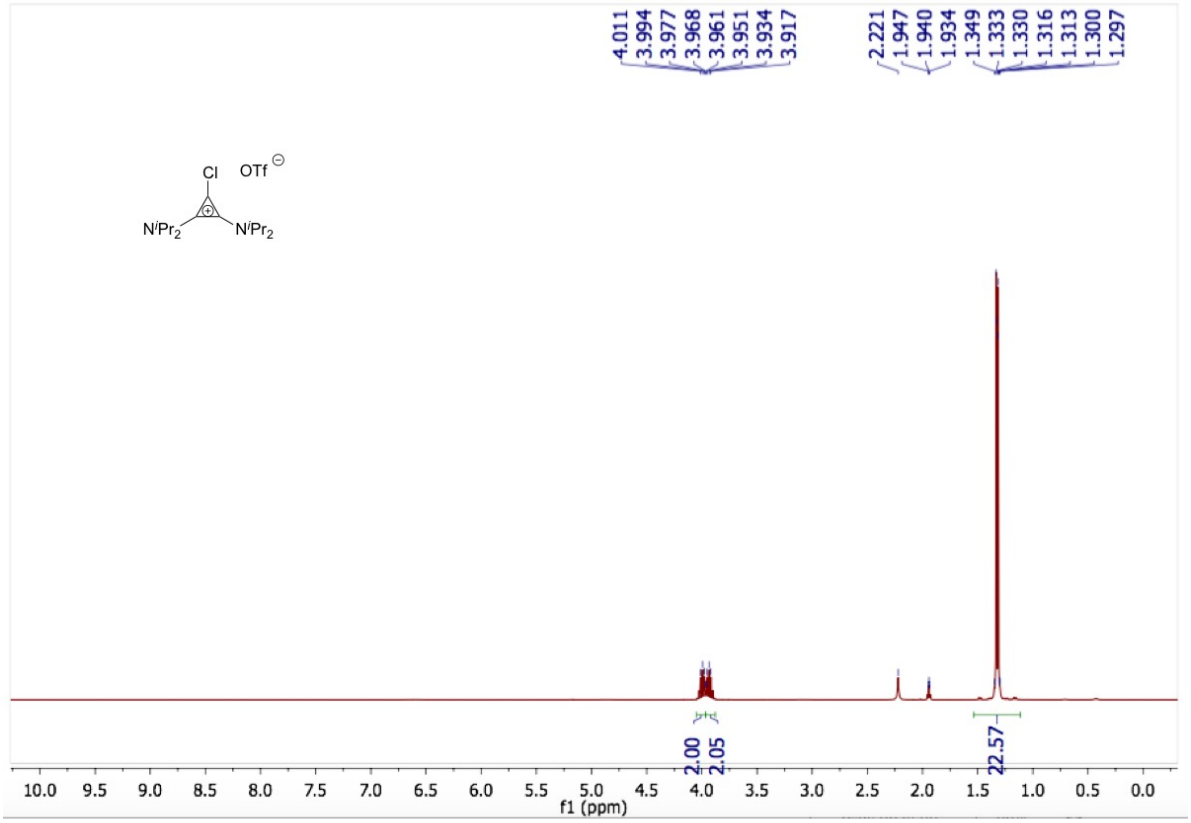

137.532
133.723
129.946
128.982
77.583
77.160
76.736
Ph
As
I
Ph
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

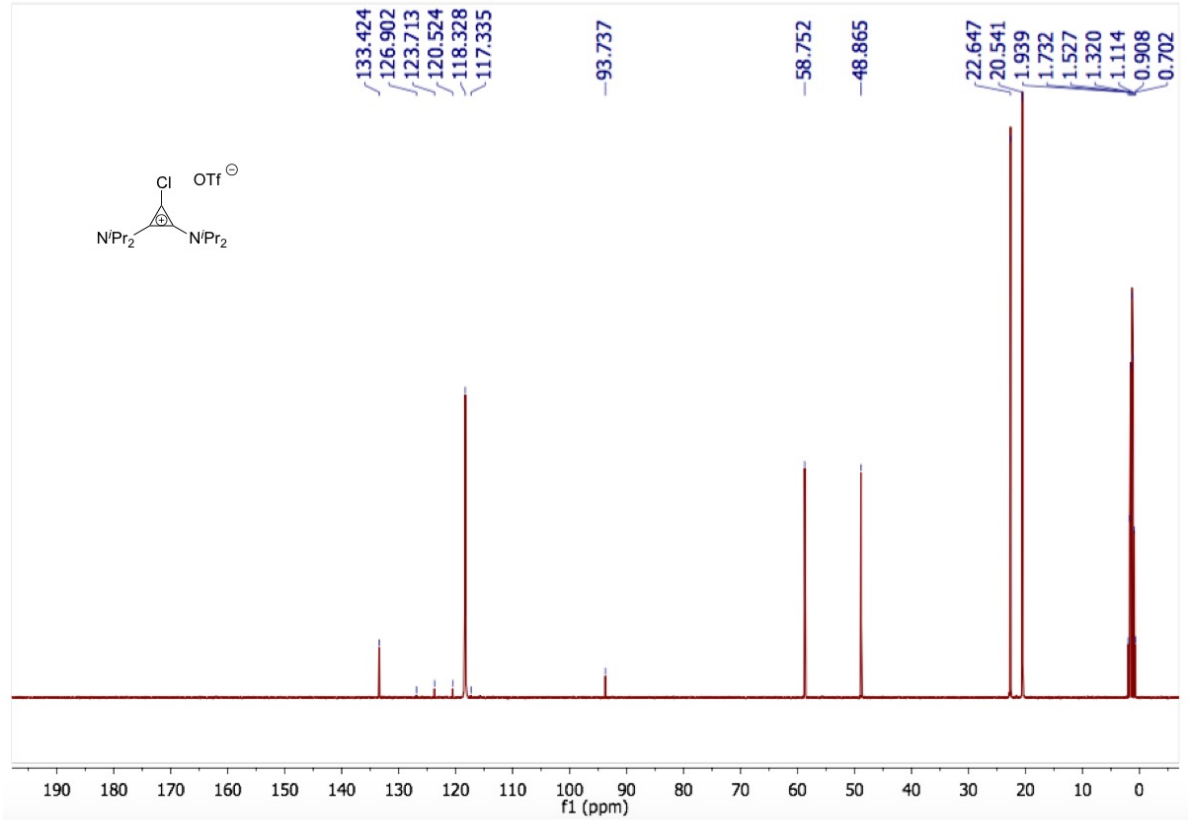

7.307
7.304
7.300
7.298
7.296
7.292
7.290
7.286
7.281
7.275
7.153
7.148
7.141
7.139
7.137
7.134
7.131
7.128
7.121
7.119
7.113
7.105
7.103
0.081
Ph
As
Ph
SiMe3
4.00
6.01
9.62
f1 (ppm)

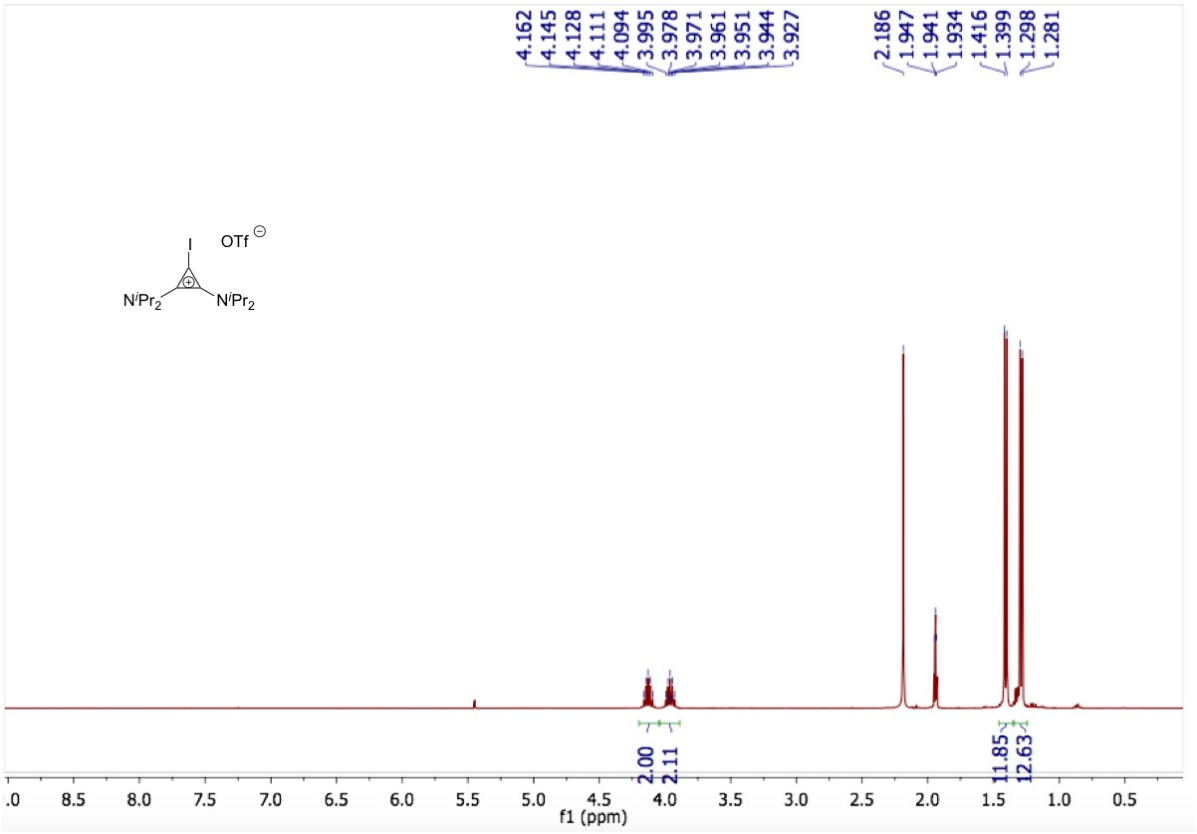

137.510
134.409
128.633
127.394
77.584
77.160
76.737
-0.276
-0.596
-0.919
Ph
As
Ph
SiMe3
f1 (ppm)

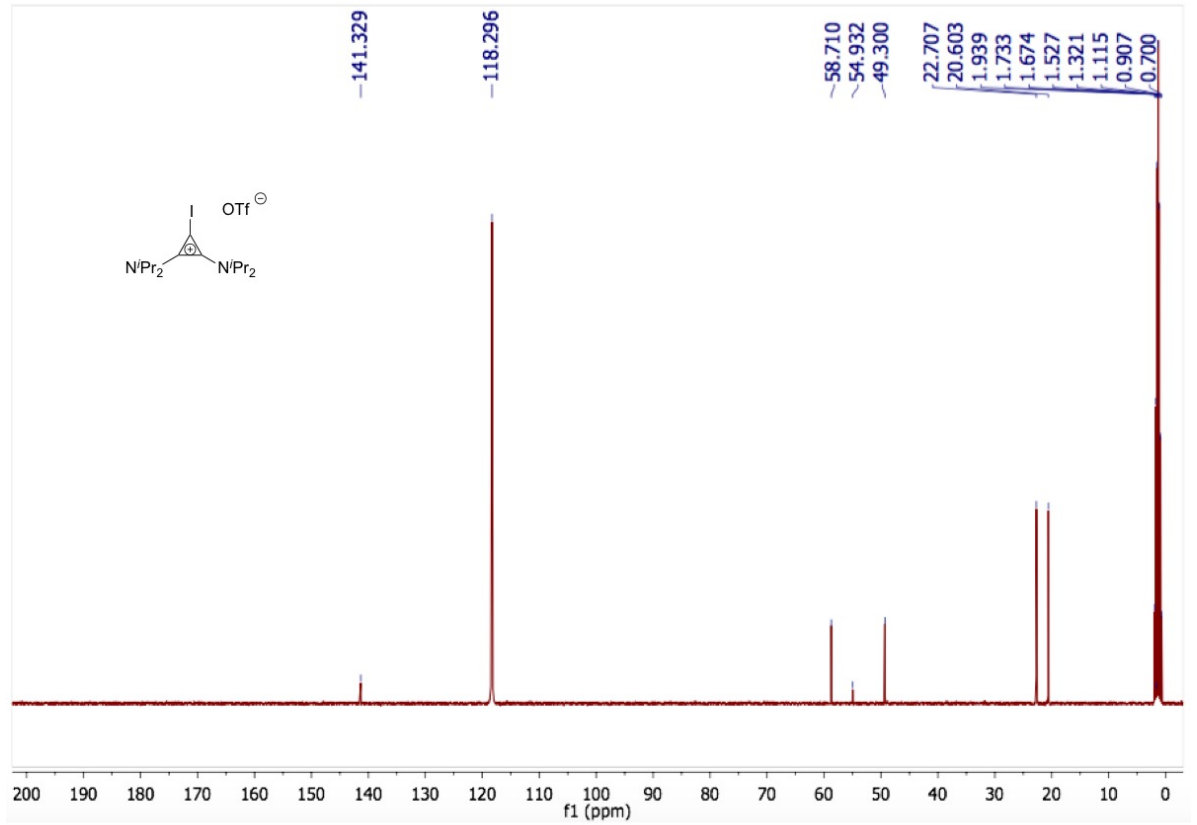

7.432
7.425
7.421
7.417
7.413
7.408
7.400
7.238
7.225
7.218
7.212
7.206
7.201
7.197
7.191
7.185
4.853
Ph
As
H
Ph
3.76
6.29
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

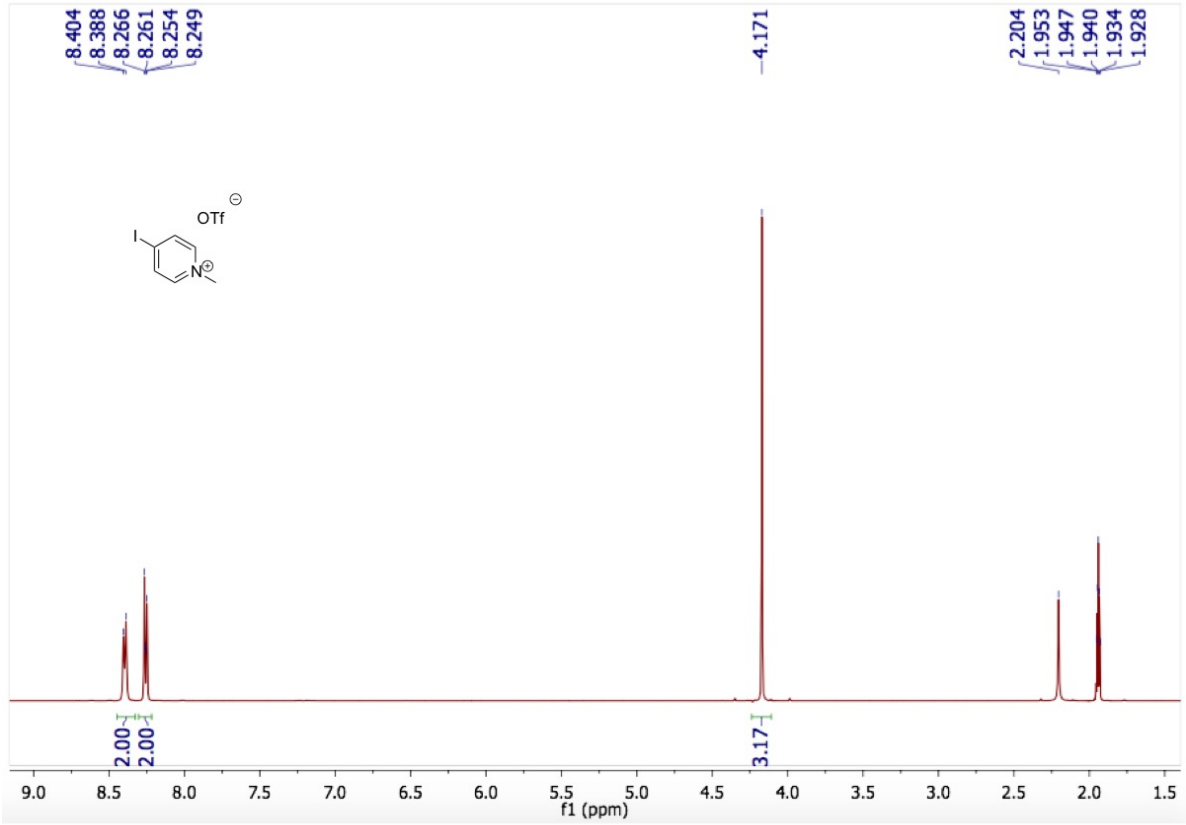

136.631
134.719
128.844
128.263
77.583
77.160
76.737
Ph
As
H
Ph
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

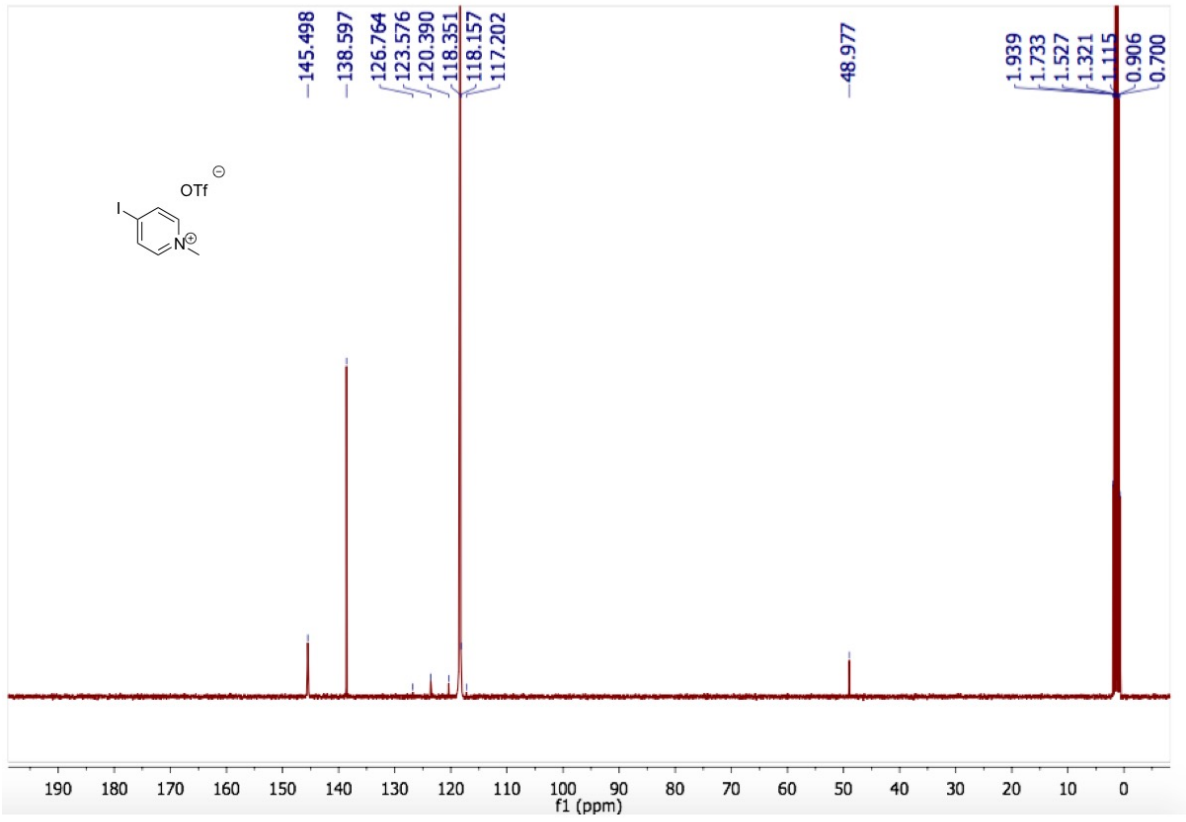

4.011
3.994
3.977
3.968
3.961
3.951
3.934
3.917
2.221
1.947
1.940
1.934
1.349
1.333
1.330
1.316
1.313
1.300
1.297
Cl
OTf
N^{i}Pr$_2$
N^{i}Pr$_2$
2.00
2.05
22.57
f1 (ppm)

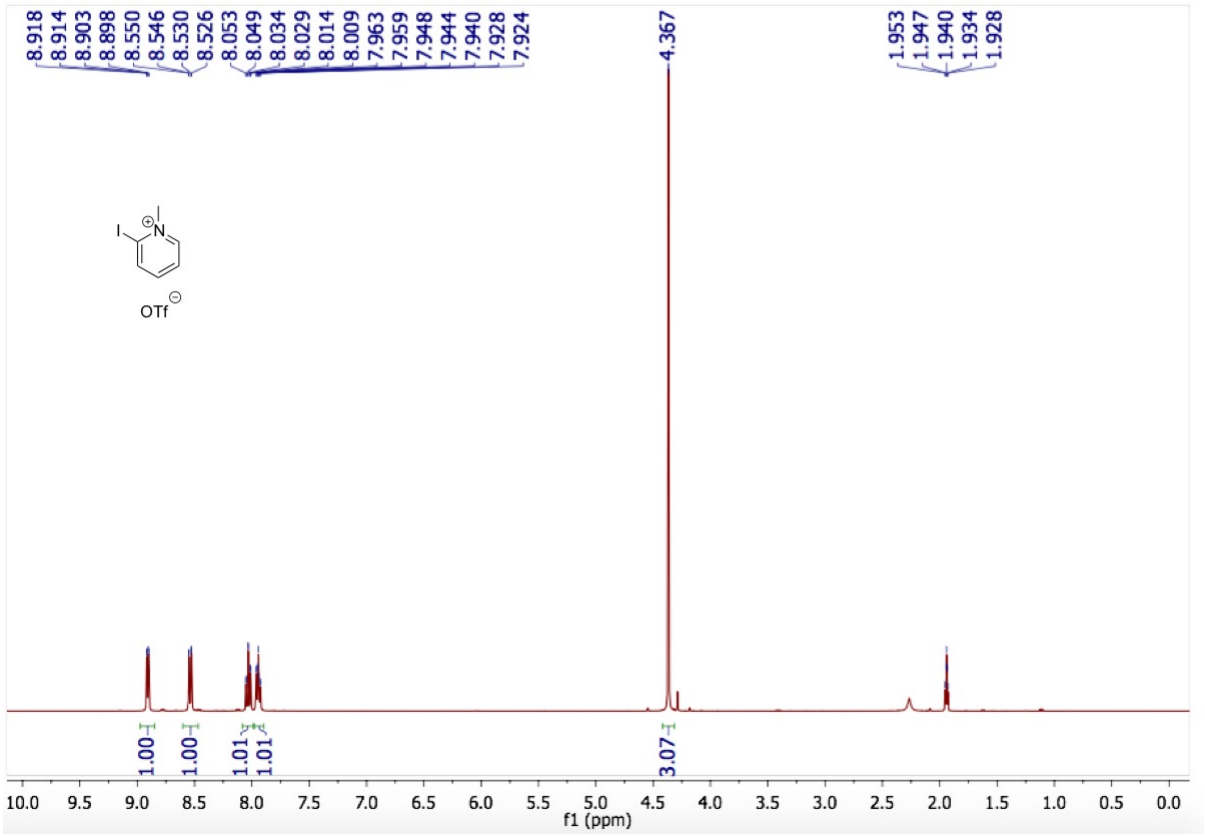

133.424
126.902
123.713
120.524
118.328
117.335
93.737
58.752
48.865
22.647
20.541
1.939
1.732
1.527
1.320
1.114
0.908
0.702
Cl
OTf
N^{i}Pr$_2$
N^{i}Pr$_2$
f1 (ppm)

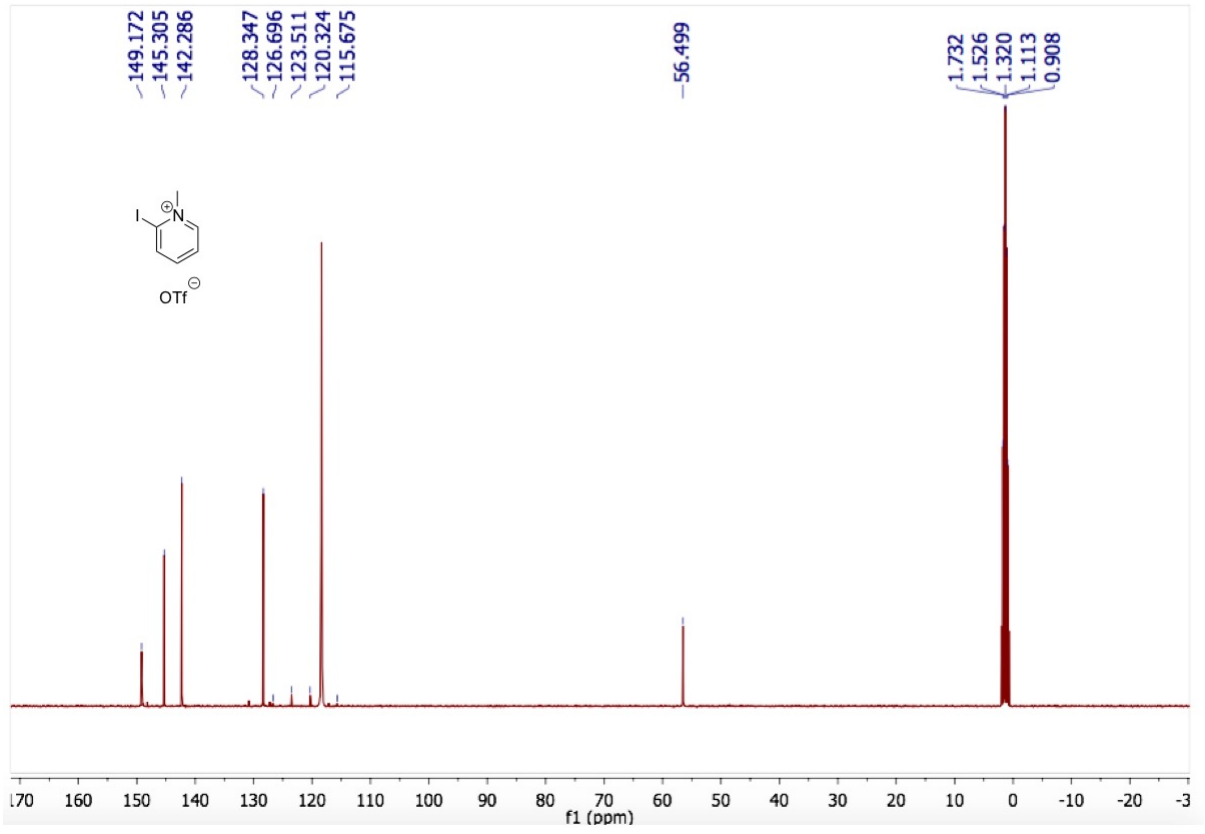

4.162
4.145
4.128
4.111
4.094
3.995
3.978
3.971
3.961
3.951
3.944
3.927
2.186
1.947
1.941
1.934
1.416
1.399
1.298
1.281
I
OTf
N^{i}Pr$_2$
N^{i}Pr$_2$
2.00
2.11
11.85
12.63
f1 (ppm)


141.329
118.296
58.710
54.932
49.300
22.707
20.603
1.939
1.733
1.674
1.527
1.321
1.115
0.907
0.700
I
OTf
N^{i}Pr$_2$
N^{i}Pr$_2$
f1 (ppm)


8.404
8.388
8.266
8.261
8.254
8.249
4.171
2.204
1.953
1.947
1.940
1.934
1.928
OTf
I
N
2.00
2.00
3.17
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5
f1 (ppm)

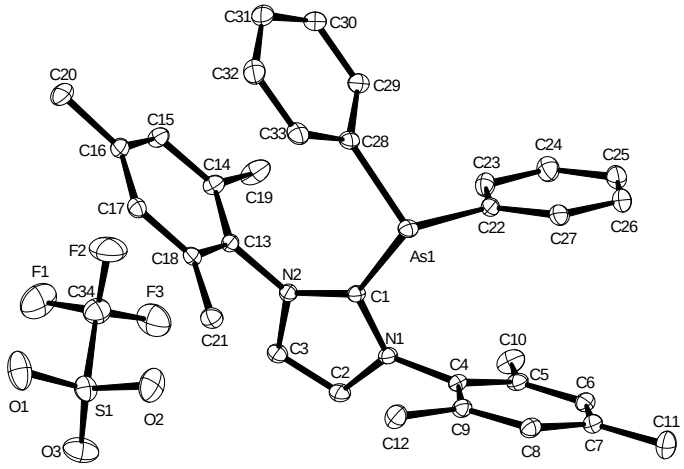

145.498
138.597
126.764
123.576
120.390
118.351
118.157
117.202
48.977
1.939
1.733
1.527
1.321
1.115
0.906
0.700
OTf
I
N
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.918
8.914
8.903
8.898
8.550
8.546
8.530
8.526
8.053
8.049
8.034
8.029
8.014
8.009
7.963
7.959
7.948
7.944
7.940
7.928
7.924
4.367
1.953
1.947
1.940
1.934
1.928
I
N
OTf
1.00
1.00
1.01
1.01
3.07
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


149.172
145.305
142.286
128.347
126.696
123.511
120.324
115.675
56.499
1.732
1.526
1.320
1.113
0.908
I
N
OTf
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -3
f1 (ppm)

4) X-ray experimental, structures, data, and parameters for reported compounds:

X-Ray diffraction analysis was performed in the department “Chemische Kristallographie” in the Max-Planck-Institut für Kohlenforschung, which is directed by Prof. Christian Lehmann. The X-ray intensity data were measured on a Bruker AXS Proteum X8 and a Bruker AXS Apex II diffractometers. These were equipped with a Cu and Mo FR591 rotating anode, respectively, and multilayer X-ray optics. The APEX2 software was used to operate both diffractometers.[14] The data were integrated with SAINT[15] and corrected for absorption effects based on Gaussian numerical integration and scaled with SADABS.[16] The crystal structures were solved by direct methods using SHELXS-97 and refined with SHELXL-2014.[17]
Ellipsoids are drawn at 50% probability, while hydrogen atoms are removed for clarity. If present all solvent molecules, disordered anions and/or organic framework are shown for a complete structural depiction.



Fully labeled solid-state structure of **3**.

Crystal data and structure refinement for 3.

CCDC	1408121	
Empirical formula	$C_{34}H_{34}AsF_3N_2O_3S$	
Color	colorless	
Formula weight	682.61 $g \cdot mol^{-1}$	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	MONOCLINIC	
Space group	p 21/n, (no. 14)	
Unit cell dimensions	a = 13.316(2) Å	α= 90°.
	b = 16.897(3) Å	β= 112.029(3)°.
	c = 15.036(3) Å	γ = 90°.
Volume	3136.2(9) $Å^3$	
Z	4	
Density (calculated)	1.446 $Mg \cdot m^{-3}$	
Absorption coefficient	1.206 mm^{-1}	
F(000)	1408 e	
Crystal size	0.26 x 0.23 x 0.16 mm^3	
θ range for data collection	2.582 to 35.630°.	
Index ranges	$-21 \le h \le 21$, $-27 \le k \le 27$, $-24 \le l \le 24$	
Reflections collected	118979	
Independent reflections	14444 [R_{int} = 0.0307]	
Reflections with I>2σ(I)	12517	
Completeness to θ = 25.242°	99.9 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.85152 and 0.72701	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	14444 / 0 / 403	
Goodness-of-fit on F^2	1.050	
Final R indices [I>2σ(I)]	R_1 = 0.0261	wR^2 = 0.0710
R indices (all data)	R_1 = 0.0336	wR^2 = 0.0745
Extinction coefficient	n/a	
Largest diff. peak and hole	0.567 and -0.343 $e \cdot Å^{-3}$	

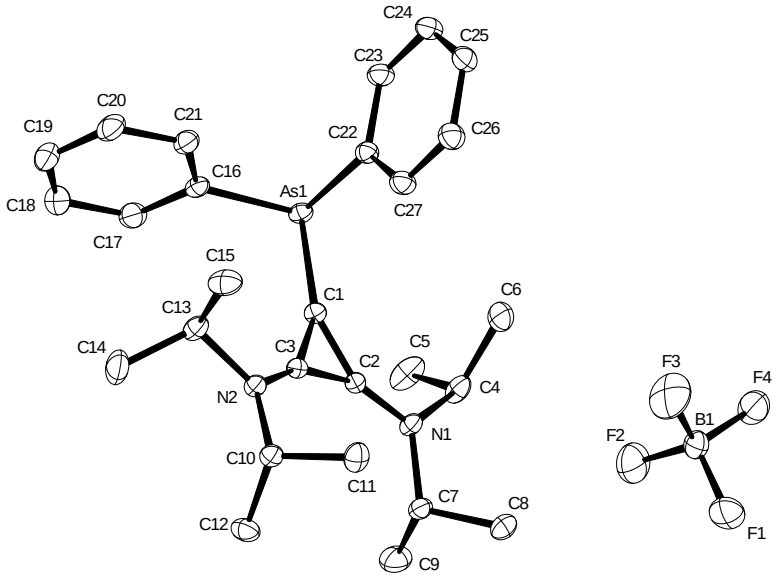
Bond lengths [Å] and angles [°] for 3.

As(1)-C(1)	1.9858(8)	As(1)-C(22)	1.9461(9)
As(1)-C(28)	1.9468(9)	C(1)-N(1)	1.3506(10)
C(1)-N(2)	1.3485(10)	C(2)-H(2)	0.9500
C(2)-C(3)	1.3539(12)	C(2)-N(1)	1.3843(11)
C(3)-H(3)	0.9500	C(3)-N(2)	1.3862(11)
C(4)-C(5)	1.3950(11)	C(4)-C(9)	1.4010(11)
C(4)-N(1)	1.4460(10)	C(5)-C(6)	1.3959(12)
C(5)-C(10)	1.5047(13)	C(6)-H(6)	0.9500
C(6)-C(7)	1.3954(13)	C(7)-C(8)	1.3934(12)
C(7)-C(11)	1.5056(13)	C(8)-H(8)	0.9500
C(8)-C(9)	1.3927(12)	C(9)-C(12)	1.5059(12)
C(10)-H(10A)	0.9800	C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800	C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800	C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800	C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800	C(13)-C(14)	1.3951(11)
C(13)-C(18)	1.3942(11)	C(13)-N(2)	1.4488(10)
C(14)-C(15)	1.3927(12)	C(14)-C(19)	1.5013(13)
C(15)-H(15)	0.9500	C(15)-C(16)	1.3926(12)
C(16)-C(17)	1.3929(12)	C(16)-C(20)	1.5057(12)
C(17)-H(17)	0.9500	C(17)-C(18)	1.3933(12)
C(18)-C(21)	1.5020(12)	C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800	C(19)-H(19C)	0.9800
C(20)-H(20A)	0.9800	C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800	C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800	C(21)-H(21C)	0.9800
C(22)-C(23)	1.3964(13)	C(22)-C(27)	1.3982(12)
C(23)-H(23)	0.9500	C(23)-C(24)	1.3921(13)
C(24)-H(24)	0.9500	C(24)-C(25)	1.3922(14)
C(25)-H(25)	0.9500	C(25)-C(26)	1.3881(16)
C(26)-H(26)	0.9500	C(26)-C(27)	1.3905(14)
C(27)-H(27)	0.9500	C(28)-C(29)	1.3962(13)
C(28)-C(33)	1.3978(12)	C(29)-H(29)	0.9500
C(29)-C(30)	1.3932(13)	C(30)-H(30)	0.9500
C(30)-C(31)	1.3898(15)	C(31)-H(31)	0.9500
C(31)-C(32)	1.3900(16)	C(32)-H(32)	0.9500

C(32)-C(33)	1.3873(13)	C(33)-H(33)	0.9500
C(34)-F(1)	1.3315(13)	C(34)-F(2)	1.3379(13)
C(34)-F(3)	1.3340(13)	C(34)-S(1)	1.8256(12)
O(1)-S(1)	1.4428(9)	O(2)-S(1)	1.4450(8)
O(3)-S(1)	1.4387(8)		

C(22)-As(1)-C(1)	96.31(3)	C(22)-As(1)-C(28)	103.14(4)
C(28)-As(1)-C(1)	101.81(3)	N(1)-C(1)-As(1)	120.99(6)
N(2)-C(1)-As(1)	132.39(6)	N(2)-C(1)-N(1)	106.46(7)
C(3)-C(2)-H(2)	126.5	C(3)-C(2)-N(1)	107.01(7)
N(1)-C(2)-H(2)	126.5	C(2)-C(3)-H(3)	126.5
C(2)-C(3)-N(2)	106.91(7)	N(2)-C(3)-H(3)	126.5
C(5)-C(4)-C(9)	122.82(7)	C(5)-C(4)-N(1)	119.72(7)
C(9)-C(4)-N(1)	117.46(7)	C(4)-C(5)-C(6)	117.20(8)
C(4)-C(5)-C(10)	122.43(8)	C(6)-C(5)-C(10)	120.36(8)
C(5)-C(6)-H(6)	119.1	C(7)-C(6)-C(5)	121.86(8)
C(7)-C(6)-H(6)	119.1	C(6)-C(7)-C(11)	121.09(8)
C(8)-C(7)-C(6)	118.76(8)	C(8)-C(7)-C(11)	120.11(8)
C(7)-C(8)-H(8)	119.2	C(9)-C(8)-C(7)	121.59(8)
C(9)-C(8)-H(8)	119.2	C(4)-C(9)-C(12)	122.72(7)
C(8)-C(9)-C(4)	117.52(8)	C(8)-C(9)-C(12)	119.75(8)
C(5)-C(10)-H(10A)	109.5	C(5)-C(10)-H(10B)	109.5
C(5)-C(10)-H(10C)	109.5	H(10A)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10C)	109.5	H(10B)-C(10)-H(10C)	109.5
C(7)-C(11)-H(11A)	109.5	C(7)-C(11)-H(11B)	109.5
C(7)-C(11)-H(11C)	109.5	H(11A)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11C)	109.5	H(11B)-C(11)-H(11C)	109.5
C(9)-C(12)-H(12A)	109.5	C(9)-C(12)-H(12B)	109.5
C(9)-C(12)-H(12C)	109.5	H(12A)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12C)	109.5	H(12B)-C(12)-H(12C)	109.5
C(14)-C(13)-N(2)	119.38(7)	C(18)-C(13)-C(14)	122.92(7)
C(18)-C(13)-N(2)	117.70(7)	C(13)-C(14)-C(19)	121.64(8)
C(15)-C(14)-C(13)	117.35(7)	C(15)-C(14)-C(19)	120.99(8)
C(14)-C(15)-H(15)	119.1	C(14)-C(15)-C(16)	121.75(8)
C(16)-C(15)-H(15)	119.1	C(15)-C(16)-C(17)	118.87(8)
C(15)-C(16)-C(20)	120.71(8)	C(17)-C(16)-C(20)	120.41(8)
C(16)-C(17)-H(17)	119.2	C(16)-C(17)-C(18)	121.50(7)
C(18)-C(17)-H(17)	119.2	C(13)-C(18)-C(21)	122.04(7)

C(17)-C(18)-C(13)	117.58(7)	C(17)-C(18)-C(21)	120.33(7)
C(14)-C(19)-H(19A)	109.5	C(14)-C(19)-H(19B)	109.5
C(14)-C(19)-H(19C)	109.5	H(19A)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19C)	109.5	H(19B)-C(19)-H(19C)	109.5
C(16)-C(20)-H(20A)	109.5	C(16)-C(20)-H(20B)	109.5
C(16)-C(20)-H(20C)	109.5	H(20A)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20C)	109.5	H(20B)-C(20)-H(20C)	109.5
C(18)-C(21)-H(21A)	109.5	C(18)-C(21)-H(21B)	109.5
C(18)-C(21)-H(21C)	109.5	H(21A)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21C)	109.5	H(21B)-C(21)-H(21C)	109.5
C(23)-C(22)-As(1)	125.34(6)	C(23)-C(22)-C(27)	119.35(8)
C(27)-C(22)-As(1)	115.31(7)	C(22)-C(23)-H(23)	119.9
C(24)-C(23)-C(22)	120.22(8)	C(24)-C(23)-H(23)	119.9
C(23)-C(24)-H(24)	120.0	C(25)-C(24)-C(23)	120.05(9)
C(25)-C(24)-H(24)	120.0	C(24)-C(25)-H(25)	120.0
C(26)-C(25)-C(24)	119.97(9)	C(26)-C(25)-H(25)	120.0
C(25)-C(26)-H(26)	119.9	C(25)-C(26)-C(27)	120.18(9)
C(27)-C(26)-H(26)	119.9	C(22)-C(27)-H(27)	119.9
C(26)-C(27)-C(22)	120.22(9)	C(26)-C(27)-H(27)	119.9
C(29)-C(28)-As(1)	126.14(6)	C(29)-C(28)-C(33)	119.52(8)
C(33)-C(28)-As(1)	114.15(7)	C(28)-C(29)-H(29)	120.1
C(30)-C(29)-C(28)	119.76(9)	C(30)-C(29)-H(29)	120.1
C(29)-C(30)-H(30)	119.7	C(31)-C(30)-C(29)	120.51(9)
C(31)-C(30)-H(30)	119.7	C(30)-C(31)-H(31)	120.2
C(30)-C(31)-C(32)	119.69(9)	C(32)-C(31)-H(31)	120.2
C(31)-C(32)-H(32)	119.9	C(33)-C(32)-C(31)	120.23(9)
C(33)-C(32)-H(32)	119.9	C(28)-C(33)-H(33)	119.9
C(32)-C(33)-C(28)	120.27(9)	C(32)-C(33)-H(33)	119.9
C(1)-N(1)-C(2)	109.78(7)	C(1)-N(1)-C(4)	124.24(7)
C(2)-N(1)-C(4)	125.55(7)	C(1)-N(2)-C(3)	109.81(7)
C(1)-N(2)-C(13)	126.66(7)	C(3)-N(2)-C(13)	123.02(7)
F(1)-C(34)-F(2)	107.35(10)	F(1)-C(34)-F(3)	107.16(9)
F(1)-C(34)-S(1)	111.92(8)	F(2)-C(34)-S(1)	111.40(8)
F(3)-C(34)-F(2)	107.06(9)	F(3)-C(34)-S(1)	111.68(8)
O(1)-S(1)-C(34)	102.85(6)	O(1)-S(1)-O(2)	114.78(5)
O(2)-S(1)-C(34)	102.08(5)	O(3)-S(1)-C(34)	103.39(5)
O(3)-S(1)-O(1)	115.87(6)	O(3)-S(1)-O(2)	115.12(6)



Fully labeled solid-state structure of **6**.

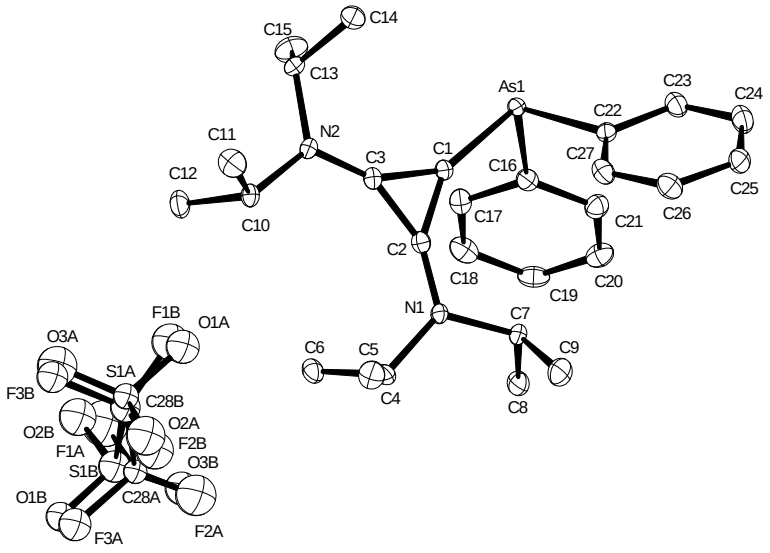
Crystal data and structure refinement of 6.

CCDC	1408070	
Empirical formula	$C_{27}H_{38}AsBF_4N_2$	
Color	colorless	
Formula weight	552.32 $g \cdot mol^{-1}$	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	MONOCLINIC	
Space group	**$P2_1/n$, (no. 14)**	
Unit cell dimensions	a = 10.043(3) Å	α= 90°.
	b = 17.936(5) Å	β= 99.492(5)°.
	c = 15.804(5) Å	γ = 90°.
Volume	2807.8(14) $Å^3$	
Z	4	
Density (calculated)	1.307 $Mg \cdot m^{-3}$	
Absorption coefficient	1.255 mm^{-1}	
F(000)	1152 e	
Crystal size	0.38 x 0.36 x 0.12 mm^3	
θ range for data collection	1.731 to 35.077°.	
Index ranges	$-16 \le h \le 16$, $-28 \le k \le 28$, $-25 \le l \le 25$	
Reflections collected	98016	
Independent reflections	12292 [R_{int} = 0.0527]	
Reflections with I>2σ(I)	9649	
Completeness to θ = 25.242°	100.0 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.86 and 0.50	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	12292 / 0 / 324	
Goodness-of-fit on F^2	1.014	
Final R indices [I>2σ(I)]	R_1 = 0.0305	wR^2 = 0.0682
R indices (all data)	R_1 = 0.0492	wR^2 = 0.0750
Largest diff. peak and hole	0.5 and -0.4 e $\cdot Å^{-3}$	

Bond lengths [Å] and angles [°] for 6.

As(1)-C(1)	1.9372(11)	As(1)-C(16)	1.9601(12)
As(1)-C(22)	1.9551(12)	F(1)-B(1)	1.3994(16)
F(2)-B(1)	1.3944(17)	F(3)-B(1)	1.3779(17)
F(4)-B(1)	1.3808(16)	N(1)-C(2)	1.3126(13)
N(1)-C(4)	1.4951(13)	N(1)-C(7)	1.4841(14)
N(2)-C(3)	1.3104(12)	N(2)-C(10)	1.4879(13)
N(2)-C(13)	1.4888(14)	C(1)-C(2)	1.3825(14)
C(1)-C(3)	1.3844(14)	C(2)-C(3)	1.4167(14)
C(4)-C(5)	1.5230(17)	C(4)-C(6)	1.5251(19)
C(7)-C(8)	1.5229(16)	C(7)-C(9)	1.5252(17)
C(10)-C(11)	1.5234(16)	C(10)-C(12)	1.5206(16)
C(13)-C(14)	1.5220(17)	C(13)-C(15)	1.5227(18)
C(16)-C(17)	1.3940(16)	C(16)-C(21)	1.3971(16)
C(17)-C(18)	1.3950(19)	C(18)-C(19)	1.388(2)
C(19)-C(20)	1.3892(19)	C(20)-C(21)	1.3949(17)
C(22)-C(23)	1.3963(15)	C(22)-C(27)	1.4006(15)
C(23)-C(24)	1.3913(17)	C(24)-C(25)	1.3873(18)
C(25)-C(26)	1.3921(17)	C(26)-C(27)	1.3901(17)
C(1)-As(1)-C(16)	98.88(4)	C(1)-As(1)-C(22)	96.92(4)
C(22)-As(1)-C(16)	100.29(5)	C(2)-N(1)-C(4)	118.32(9)
C(2)-N(1)-C(7)	121.75(8)	C(7)-N(1)-C(4)	119.25(9)
C(3)-N(2)-C(10)	122.37(9)	C(3)-N(2)-C(13)	117.64(8)
C(10)-N(2)-C(13)	119.58(8)	C(2)-C(1)-As(1)	145.71(8)
C(2)-C(1)-C(3)	61.60(7)	C(3)-C(1)-As(1)	152.66(8)
N(1)-C(2)-C(1)	147.40(9)	N(1)-C(2)-C(3)	153.17(9)
C(1)-C(2)-C(3)	59.27(7)	N(2)-C(3)-C(1)	146.87(10)
N(2)-C(3)-C(2)	153.95(10)	C(1)-C(3)-C(2)	59.14(7)
N(1)-C(4)-C(5)	111.03(10)	N(1)-C(4)-C(6)	110.62(9)
C(5)-C(4)-C(6)	112.51(10)	N(1)-C(7)-C(8)	111.26(9)
N(1)-C(7)-C(9)	111.14(9)	C(8)-C(7)-C(9)	111.82(10)
N(2)-C(10)-C(11)	111.02(8)	N(2)-C(10)-C(12)	111.22(9)
C(12)-C(10)-C(11)	113.60(10)	N(2)-C(13)-C(14)	111.08(10)
N(2)-C(13)-C(15)	110.83(10)	C(14)-C(13)-C(15)	112.98(10)
C(17)-C(16)-As(1)	116.94(9)	C(17)-C(16)-C(21)	119.92(11)
C(21)-C(16)-As(1)	123.15(8)	C(16)-C(17)-C(18)	119.87(12)

C(19)-C(18)-C(17)	120.06(12)	C(18)-C(19)-C(20)	120.30(12)
C(19)-C(20)-C(21)	119.95(12)	C(20)-C(21)-C(16)	119.87(11)
C(23)-C(22)-As(1)	116.48(8)	C(23)-C(22)-C(27)	119.31(10)
C(27)-C(22)-As(1)	124.17(8)	C(24)-C(23)-C(22)	120.26(10)
C(25)-C(24)-C(23)	120.02(11)	C(24)-C(25)-C(26)	120.27(11)
C(27)-C(26)-C(25)	119.85(11)	C(26)-C(27)-C(22)	120.28(10)
F(2)-B(1)-F(1)	109.60(11)	F(3)-B(1)-F(1)	109.99(11)
F(3)-B(1)-F(2)	108.49(11)	F(3)-B(1)-F(4)	109.60(12)
F(4)-B(1)-F(1)	109.11(11)	F(4)-B(1)-F(2)	110.03(11)



Fully labeled solid-state structure of **7**.

Crystal data and structure refinement for 7.

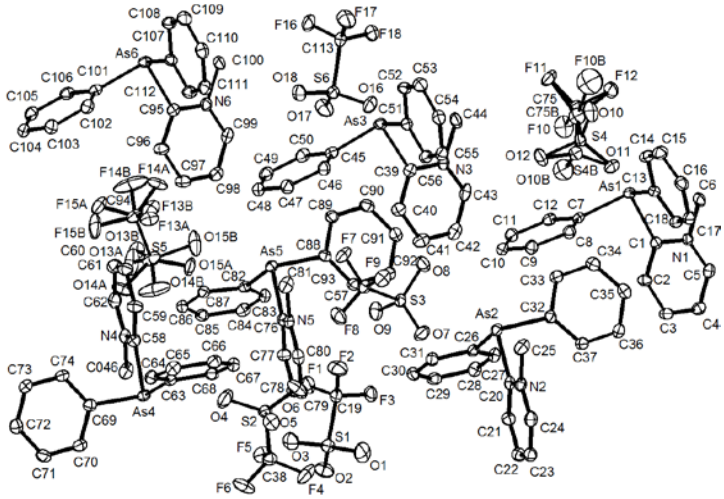
CCDC	1408081	
Empirical formula	$C_{28}H_{38}AsF_3N_2O_3S$	
Color	colorless	
Formula weight	614.58 g·mol^{-1}	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	TRICLINIC	
Space group	**P$\bar{1}$, (no. 2)**	
Unit cell dimensions	a = 10.6351(12) Å	α= 90.829(2)°.
	b = 11.0543(12) Å	β= 91.816(2)°.
	c = 12.4299(14) Å	γ = 93.933(2)°.
Volume	1456.9(3) Å^3	
Z	2	
Density (calculated)	1.401 Mg · m^{-3}	
Absorption coefficient	1.289 mm^{-1}	
F(000)	640 e	
Crystal size	0.12 x 0.10 x 0.06 mm^3	
θ range for data collection	1.639 to 30.995°.	
Index ranges	-15 ≤ h ≤ 15, -15≤ k ≤ 15, -17 ≤ l ≤ 17	
Reflections collected	43067	
Independent reflections	9200 [R_{int} = 0.0586]	
Reflections with I>2σ(I)	8090	
Completeness to θ = 25.242°	100.0 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.93 and 0.85	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9200 / 0 / 343	
Goodness-of-fit on F^2	1.255	
Final R indices [I>2σ(I)]	R_1 = 0.0559	wR^2 = 0.1288
R indices (all data)	R_1 = 0.0654	wR^2 = 0.1369
Largest diff. peak and hole	1.1 and -1.1 e · Å^{-3}	

Bond lengths [Å] and angles [°] for 7.

As(1)-C(1)	1.941(3)	As(1)-C(16)	1.966(3)
As(1)-C(22)	1.958(3)	S(1A)-O(1A)	1.372(9)
S(1A)-O(2A)	1.298(10)	S(1A)-O(3A)	1.323(10)
S(1A)-C(28A)	1.946(8)	S(1B)-O(1B)	1.338(7)
S(1B)-O(2B)	1.398(9)	S(1B)-O(3B)	1.290(7)
S(1B)-C(28B)	1.757(11)	F(1A)-C(28A)	1.562(12)
F(1B)-C(28B)	1.419(13)	F(2A)-C(28A)	1.156(10)
F(2B)-C(28B)	1.450(13)	F(3A)-C(28A)	1.439(9)
F(3B)-C(28B)	1.487(12)	N(1)-C(2)	1.302(4)
N(1)-C(4)	1.485(4)	N(1)-C(7)	1.486(4)
N(2)-C(3)	1.304(4)	N(2)-C(10)	1.485(4)
N(2)-C(13)	1.489(4)	C(1)-C(2)	1.382(4)
C(1)-C(3)	1.382(4)	C(2)-C(3)	1.420(4)
C(4)-C(5)	1.524(4)	C(4)-C(6)	1.523(4)
C(7)-C(8)	1.519(4)	C(7)-C(9)	1.522(4)
C(10)-C(11)	1.525(4)	C(10)-C(12)	1.516(4)
C(13)-C(14)	1.522(5)	C(13)-C(15)	1.522(5)
C(16)-C(17)	1.407(4)	C(16)-C(21)	1.388(4)
C(17)-C(18)	1.390(5)	C(18)-C(19)	1.390(5)
C(19)-C(20)	1.383(5)	C(20)-C(21)	1.403(5)
C(22)-C(23)	1.396(4)	C(22)-C(27)	1.390(4)
C(23)-C(24)	1.387(5)	C(24)-C(25)	1.392(5)
C(25)-C(26)	1.389(5)	C(26)-C(27)	1.387(5)

C(1)-As(1)-C(16)	93.35(13)	C(1)-As(1)-C(22)	97.63(13)
C(22)-As(1)-C(16)	100.53(13)	O(1A)-S(1A)-C(28A)	100.2(5)
O(2A)-S(1A)-O(1A)	110.8(6)	O(2A)-S(1A)-O(3A)	121.7(6)
O(2A)-S(1A)-C(28A)	101.2(5)	O(3A)-S(1A)-O(1A)	113.0(6)
O(3A)-S(1A)-C(28A)	106.7(5)	O(1B)-S(1B)-O(2B)	104.2(5)
O(1B)-S(1B)-C(28B)	105.3(5)	O(2B)-S(1B)-C(28B)	100.9(5)
O(3B)-S(1B)-O(1B)	121.4(5)	O(3B)-S(1B)-O(2B)	115.8(5)
O(3B)-S(1B)-C(28B)	107.0(5)	C(2)-N(1)-C(4)	123.2(2)
C(2)-N(1)-C(7)	117.3(2)	C(4)-N(1)-C(7)	119.5(2)
C(3)-N(2)-C(10)	120.7(3)	C(3)-N(2)-C(13)	119.4(2)

C(10)-N(2)-C(13)	119.9(2)	C(2)-C(1)-As(1)	147.8(2)
C(3)-C(1)-As(1)	149.2(2)	C(3)-C(1)-C(2)	61.8(2)
N(1)-C(2)-C(1)	145.9(3)	N(1)-C(2)-C(3)	155.1(3)
C(1)-C(2)-C(3)	59.1(2)	N(2)-C(3)-C(1)	149.5(3)
N(2)-C(3)-C(2)	151.4(3)	C(1)-C(3)-C(2)	59.1(2)
N(1)-C(4)-C(5)	111.6(3)	N(1)-C(4)-C(6)	111.3(3)
C(6)-C(4)-C(5)	113.9(3)	N(1)-C(7)-C(8)	111.5(2)
N(1)-C(7)-C(9)	110.6(3)	C(8)-C(7)-C(9)	112.3(3)
N(2)-C(10)-C(11)	110.5(3)	N(2)-C(10)-C(12)	111.1(3)
C(12)-C(10)-C(11)	112.8(3)	N(2)-C(13)-C(14)	110.7(3)
N(2)-C(13)-C(15)	110.8(3)	C(14)-C(13)-C(15)	112.5(3)
C(17)-C(16)-As(1)	117.3(2)	C(21)-C(16)-As(1)	124.0(2)
C(21)-C(16)-C(17)	118.5(3)	C(18)-C(17)-C(16)	120.7(3)
C(19)-C(18)-C(17)	120.2(3)	C(20)-C(19)-C(18)	119.6(3)
C(19)-C(20)-C(21)	120.4(3)	C(16)-C(21)-C(20)	120.5(3)
C(23)-C(22)-As(1)	116.9(2)	C(27)-C(22)-As(1)	123.8(2)
C(27)-C(22)-C(23)	119.2(3)	C(24)-C(23)-C(22)	120.3(3)
C(23)-C(24)-C(25)	120.3(3)	C(26)-C(25)-C(24)	119.2(3)
C(27)-C(26)-C(25)	120.7(3)	C(26)-C(27)-C(22)	120.2(3)
F(1A)-C(28A)-S(1A)	99.2(5)	F(2A)-C(28A)-S(1A)	115.4(7)
F(2A)-C(28A)-F(1A)	113.5(7)	F(2A)-C(28A)-F(3A)	118.5(7)
F(3A)-C(28A)-S(1A)	103.7(5)	F(3A)-C(28A)-F(1A)	104.3(7)
F(1B)-C(28B)-S(1B)	112.4(7)	F(1B)-C(28B)-F(2B)	111.9(8)
F(1B)-C(28B)-F(3B)	105.2(8)	F(2B)-C(28B)-S(1B)	110.7(7)
F(2B)-C(28B)-F(3B)	102.2(7)	F(3B)-C(28B)-S(1B)	113.8(7)



Fully labeled solid-state structure of **11**.

Crystal data and structure refinement for 11.

CCDC	1472100	
Empirical formula	$C_{19}H_{17}AsF_3NO_3S$	
Color	colourless	
Formula weight	471.32 g·mol^{-1}	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	triclinic	
Space group	*P* 1, (no. 2)	
Unit cell dimensions	a = 15.894(3) Å	α= 90.069(3)°.
	b = 18.959(3) Å	β= 95.311(3)°.
	c = 19.090(3) Å	γ = 90.042(3)°.
Volume	5727.5(16) Å^3	
Z	12	
Density (calculated)	1.640 Mg·m^{-3}	
Absorption coefficient	1.939 mm^{-1}	
F(000)	2856 e	
Crystal size	0.240 x 0.235 x 0.123 mm^3	
θ range for data collection	2.812 to 33.626°.	
Index ranges	-24 ≤ h ≤ 24, -29≤ k ≤ 29, -29≤ l ≤ 29	
Reflections collected	198347	
Independent reflections	45152 [R_{int} = 0.0498]	
Reflections with I>2σ(I)	37747	
Completeness to θ = 25.242°	99.8 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.84087 and 0.68132	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	45152 / 0 / 1591	
Goodness-of-fit on F^2	0.980	
Final R indices [I>2σ(I)]	R_1 = 0.0361	wR^2 = 0.0820
R indices (all data)	R_1 = 0.0512	wR^2 = 0.0884
Extinction coefficient	0	
Largest diff. peak and hole	1.471 and -0.669 e·Å^{-3}	
Twinning law	[1 0 0 0 1 0 0 0 1]	
Batch scale factor	0.3329(4)	

Bond lengths [Å] and angles [°] for 11.

C(1)-N(1)	1.360(3)	C(1)-C(2)	1.379(3)
C(1)-As(1)	1.992(2)	C(2)-C(3)	1.392(3)
C(2)-H(2)	0.9500	C(3)-C(4)	1.378(3)
C(3)-H(3)	0.9500	C(4)-C(5)	1.369(3)
C(4)-H(4)	0.9500	C(5)-N(1)	1.349(3)
C(5)-H(5)	0.9500	C(6)-N(1)	1.477(3)
C(6)-H(6A)	0.9800	C(6)-H(6B)	0.9800
C(6)-H(6C)	0.9800	C(7)-C(12)	1.395(3)
C(7)-C(8)	1.397(3)	C(7)-As(1)	1.952(2)
C(8)-C(9)	1.391(3)	C(8)-H(8)	0.9500
C(9)-C(10)	1.382(3)	C(9)-H(9)	0.9500
C(10)-C(11)	1.399(3)	C(10)-H(10)	0.9500
C(11)-C(12)	1.388(3)	C(11)-H(11)	0.9500
C(12)-H(12)	0.9500	C(13)-C(18)	1.388(3)
C(13)-C(14)	1.402(3)	C(13)-As(1)	1.954(2)
C(14)-C(15)	1.387(3)	C(14)-H(14)	0.9500
C(15)-C(16)	1.381(3)	C(15)-H(15)	0.9500
C(16)-C(17)	1.382(3)	C(16)-H(16)	0.9500
C(17)-C(18)	1.393(3)	C(17)-H(17)	0.9500
C(18)-H(18)	0.9500	C(19)-F(1)	1.322(3)
C(19)-F(3)	1.334(3)	C(19)-F(2)	1.338(3)
C(19)-S(1)	1.826(2)	C(20)-N(2)	1.361(3)
C(20)-C(21)	1.392(3)	C(20)-As(2)	1.986(2)
C(21)-C(22)	1.383(3)	C(21)-H(21)	0.9500
C(22)-C(23)	1.389(3)	C(22)-H(22)	0.9500
C(23)-C(24)	1.373(3)	C(23)-H(23)	0.9500
C(24)-N(2)	1.352(3)	C(24)-H(24)	0.9500
C(25)-N(2)	1.479(3)	C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800	C(25)-H(25C)	0.9800
C(26)-C(27)	1.395(3)	C(26)-C(31)	1.401(3)
C(26)-As(2)	1.955(2)	C(27)-C(28)	1.390(3)
C(27)-H(27)	0.9500	C(28)-C(29)	1.387(3)
C(28)-H(28)	0.9500	C(29)-C(30)	1.389(3)
C(29)-H(29)	0.9500	C(30)-C(31)	1.385(3)
C(30)-H(30)	0.9500	C(31)-H(31)	0.9500
C(32)-C(37)	1.389(3)	C(32)-C(33)	1.401(3)
C(32)-As(2)	1.953(2)	C(33)-C(34)	1.387(3)

C(33)-H(33)	0.9500	C(34)-C(35)	1.388(3)
C(34)-H(34)	0.9500	C(35)-C(36)	1.391(3)
C(35)-H(35)	0.9500	C(36)-C(37)	1.386(3)
C(36)-H(36)	0.9500	C(37)-H(37)	0.9500
C(38)-F(4)	1.325(3)	C(38)-F(6)	1.329(3)
C(38)-F(5)	1.332(2)	C(38)-S(2)	1.821(2)
C(39)-N(3)	1.364(3)	C(39)-C(40)	1.376(3)
C(39)-As(3)	1.990(2)	C(40)-C(41)	1.393(3)
C(40)-H(40)	0.9500	C(41)-C(42)	1.381(3)
C(41)-H(41)	0.9500	C(42)-C(43)	1.373(3)
C(42)-H(42)	0.9500	C(43)-N(3)	1.352(3)
C(43)-H(43)	0.9500	C(44)-N(3)	1.477(3)
C(44)-H(44A)	0.9800	C(44)-H(44B)	0.9800
C(44)-H(44C)	0.9800	C(45)-C(46)	1.395(3)
C(45)-C(50)	1.395(3)	C(45)-As(3)	1.948(2)
C(046)-N(4)	1.481(3)	C(046)-H(04A)	0.9800
C(046)-H(04B)	0.9800	C(046)-H(04C)	0.9800
C(46)-C(47)	1.396(3)	C(46)-H(46)	0.9500
C(47)-C(48)	1.382(3)	C(47)-H(47)	0.9500
C(48)-C(49)	1.392(3)	C(48)-H(48)	0.9500
C(49)-C(50)	1.392(3)	C(49)-H(49)	0.9500
C(50)-H(50)	0.9500	C(51)-C(56)	1.390(3)
C(51)-C(52)	1.399(3)	C(51)-As(3)	1.956(2)
C(52)-C(53)	1.392(3)	C(52)-H(52)	0.9500
C(53)-C(54)	1.379(3)	C(53)-H(53)	0.9500
C(54)-C(55)	1.398(3)	C(54)-H(54)	0.9500
C(55)-C(56)	1.391(3)	C(55)-H(55)	0.9500
C(56)-H(56)	0.9500	C(57)-F(7)	1.328(2)
C(57)-F(8)	1.332(2)	C(57)-F(9)	1.337(2)
C(57)-S(3)	1.823(2)	C(58)-N(4)	1.358(3)
C(58)-C(59)	1.393(3)	C(58)-As(4)	1.980(2)
C(59)-C(60)	1.388(3)	C(59)-H(59)	0.9500
C(60)-C(61)	1.384(3)	C(60)-H(60)	0.9500
C(61)-C(62)	1.385(3)	C(61)-H(61)	0.9500
C(62)-N(4)	1.348(3)	C(62)-H(62)	0.9500
C(63)-C(64)	1.397(3)	C(63)-C(68)	1.401(3)
C(63)-As(4)	1.954(2)	C(64)-C(65)	1.387(3)
C(64)-H(64)	0.9500	C(65)-C(66)	1.388(3)

C(65)-H(65)	0.9500	C(66)-C(67)	1.391(3)
C(66)-H(66)	0.9500	C(67)-C(68)	1.386(3)
C(67)-H(67)	0.9500	C(68)-H(68)	0.9500
C(69)-C(74)	1.395(3)	C(69)-C(70)	1.400(3)
C(69)-As(4)	1.955(2)	C(70)-C(71)	1.389(3)
C(70)-H(70)	0.9500	C(71)-C(72)	1.387(3)
C(71)-H(71)	0.9500	C(72)-C(73)	1.394(3)
C(72)-H(72)	0.9500	C(73)-C(74)	1.385(3)
C(73)-H(73)	0.9500	C(74)-H(74)	0.9500
C(75)-C(75B)	0.58(4)	C(75)-F(11)	1.321(3)
C(75)-F(12)	1.326(3)	C(75)-F(10)	1.334(3)
C(75)-S(4B)	1.810(7)	C(75)-S(4)	1.821(3)
C(75)-F(10B)	1.90(3)	C(75B)-S(4)	1.25(4)
C(75B)-S(4B)	1.31(4)	C(75B)-F(11)	1.61(4)
C(75B)-F(12)	1.62(4)	C(75B)-F(10)	1.65(4)
C(75B)-F(10B)	1.70(5)	C(76)-N(5)	1.357(3)
C(76)-C(77)	1.389(3)	C(76)-As(5)	1.989(2)
C(77)-C(78)	1.384(3)	C(77)-H(77)	0.9500
C(78)-C(79)	1.381(3)	C(78)-H(78)	0.9500
C(79)-C(80)	1.374(3)	C(79)-H(79)	0.9500
C(80)-N(5)	1.354(3)	C(80)-H(80)	0.9500
C(81)-N(5)	1.480(3)	C(81)-H(81A)	0.9800
C(81)-H(81B)	0.9800	C(81)-H(81C)	0.9800
C(82)-C(87)	1.392(3)	C(82)-C(83)	1.397(3)
C(82)-As(5)	1.950(2)	C(83)-C(84)	1.386(3)
C(83)-H(83)	0.9500	C(84)-C(85)	1.388(3)
C(84)-H(84)	0.9500	C(85)-C(86)	1.392(3)
C(85)-H(85)	0.9500	C(86)-C(87)	1.387(3)
C(86)-H(86)	0.9500	C(87)-H(87)	0.9500
C(88)-C(93)	1.394(3)	C(88)-C(89)	1.397(3)
C(88)-As(5)	1.954(2)	C(89)-C(90)	1.389(3)
C(89)-H(89)	0.9500	C(90)-C(91)	1.388(3)
C(90)-H(90)	0.9500	C(91)-C(92)	1.394(3)
C(91)-H(91)	0.9500	C(92)-C(93)	1.391(3)
C(92)-H(92)	0.9500	C(93)-H(93)	0.9500
C(94)-F(15A)	1.245(4)	C(94)-F(14B)	1.252(4)
C(94)-F(13B)	1.322(14)	C(94)-F(13A)	1.323(13)
C(94)-F(14A)	1.424(4)	C(94)-F(15B)	1.434(4)

C(94)-S(5)	1.806(2)	C(95)-N(6)	1.362(3)
C(95)-C(96)	1.383(3)	C(95)-As(6)	1.993(2)
C(96)-C(97)	1.398(3)	C(96)-H(96)	0.9500
C(97)-C(98)	1.379(3)	C(97)-H(97)	0.9500
C(98)-C(99)	1.368(3)	C(98)-H(98)	0.9500
C(99)-N(6)	1.354(3)	C(99)-H(99)	0.9500
C(100)-N(6)	1.490(3)	C(100)-H(10A)	0.9800
C(100)-H(10B)	0.9800	C(100)-H(10C)	0.9800
C(101)-C(106)	1.391(3)	C(101)-C(102)	1.393(3)
C(101)-As(6)	1.957(2)	C(102)-C(103)	1.394(3)
C(102)-H(102)	0.9500	C(103)-C(104)	1.382(3)
C(103)-H(103)	0.9500	C(104)-C(105)	1.388(3)
C(104)-H(104)	0.9500	C(105)-C(106)	1.392(3)
C(105)-H(105)	0.9500	C(106)-H(106)	0.9500
C(107)-C(112)	1.392(3)	C(107)-C(108)	1.402(3)
C(107)-As(6)	1.951(2)	C(108)-C(109)	1.396(3)
C(108)-H(108)	0.9500	C(109)-C(110)	1.381(3)
C(109)-H(109)	0.9500	C(110)-C(111)	1.393(3)
C(110)-H(110)	0.9500	C(111)-C(112)	1.394(3)
C(111)-H(111)	0.9500	C(112)-H(112)	0.9500
C(113)-F(16)	1.330(3)	C(113)-F(18)	1.335(3)
C(113)-F(17)	1.342(3)	C(113)-S(6)	1.820(2)
O(1)-S(1)	1.4340(19)	O(2)-S(1)	1.430(2)
O(3)-S(1)	1.4490(19)	O(4)-S(2)	1.437(2)
O(5)-S(2)	1.4388(17)	O(6)-S(2)	1.4341(2)
O(7)-S(3)	1.4436(17)	O(8)-S(3)	1.439(2)
O(9)-S(3)	1.4462(17)	O(10)-F(10B)	1.32(3)
O(10)-S(4)	1.4384(19)	O(10)-S(4B)	2.145(10)
O(10B)-S(4B)	1.47(3)	O(10B)-F(10)	1.60(3)
O(10B)-S(4)	2.16(3)	O(11)-S(4B)	1.293(8)
O(11)-S(4)	1.4288(18)	O(12)-S(4B)	1.329(8)
O(12)-S(4)	1.4488(17)	O(13A)-O(13B)	0.552(7)
O(13A)-S(5)	1.280(6)	O(13B)-S(5)	1.542(5)
O(14A)-O(14B)	1.184(6)	O(14A)-S(5)	1.517(3)
O(14B)-S(5)	1.453(4)	O(14B)-O(15A)	1.638(7)
O(16)-S(6)	1.4322(19)	O(15A)-O(15B)	0.886(6)
O(15A)-S(5)	1.315(4)	O(15B)-S(5)	1.548(4)
O(17)-S(6)	1.4368(18)	O(18)-S(6)	1.4418(17)

F(10B)-S(4)	1.97(3)	F(14A)-F(14B)	0.903(6)
F(14B)-F(15A)	1.399(6)	F(15A)-F(15B)	0.851(4)
S(4)-S(4B)	0.707(9)		

N(1)-C(1)-C(2)	118.24(18)	N(1)-C(1)-As(1)	118.3(2)
C(2)-C(1)-As(1)	123.47(15)	C(1)-C(2)-C(3)	121.0(2)
C(1)-C(2)-H(2)	119.5	C(3)-C(2)-H(2)	119.5
C(4)-C(3)-C(2)	118.57(19)	C(4)-C(3)-H(3)	120.7
C(2)-C(3)-H(3)	120.7	C(5)-C(4)-C(3)	119.9(2)
C(5)-C(4)-H(4)	120.1	C(3)-C(4)-H(4)	120.1
N(1)-C(5)-C(4)	120.46(19)	N(1)-C(5)-H(5)	119.8
C(4)-C(5)-H(5)	119.8	N(1)-C(6)-H(6A)	109.5
N(1)-C(6)-H(6B)	109.5	H(6A)-C(6)-H(6B)	109.5
N(1)-C(6)-H(6C)	109.5	H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5	C(12)-C(7)-C(8)	119.3(2)
C(12)-C(7)-As(1)	116.20(15)	C(8)-C(7)-As(1)	124.5(2)
C(9)-C(8)-C(7)	119.9(2)	C(9)-C(8)-H(8)	120.1
C(7)-C(8)-H(8)	120.1	C(10)-C(9)-C(8)	120.8(2)
C(10)-C(9)-H(9)	119.6	C(8)-C(9)-H(9)	119.6
C(9)-C(10)-C(11)	119.5(2)	C(9)-C(10)-H(10)	120.2
C(11)-C(10)-H(10)	120.2	C(12)-C(11)-C(10)	119.8(2)
C(12)-C(11)-H(11)	120.1	C(10)-C(11)-H(11)	120.1
C(11)-C(12)-C(7)	120.6(2)	C(11)-C(12)-H(12)	119.7
C(7)-C(12)-H(12)	119.7	C(18)-C(13)-C(14)	118.6(2)
C(18)-C(13)-As(1)	126.10(15)	C(14)-C(13)-As(1)	115.2(2)
C(15)-C(14)-C(13)	120.8(2)	C(15)-C(14)-H(14)	119.6
C(13)-C(14)-H(14)	119.6	C(16)-C(15)-C(14)	120.0(2)
C(16)-C(15)-H(15)	120.0	C(14)-C(15)-H(15)	120.0
C(15)-C(16)-C(17)	119.9(2)	C(15)-C(16)-H(16)	120.1
C(17)-C(16)-H(16)	120.1	C(16)-C(17)-C(18)	120.4(2)
C(16)-C(17)-H(17)	119.8	C(18)-C(17)-H(17)	119.8
C(13)-C(18)-C(17)	120.37(2)	C(13)-C(18)-H(18)	119.8
C(17)-C(18)-H(18)	119.8	F(1)-C(19)-F(3)	107.6(2)
F(1)-C(19)-F(2)	108.09(2)	F(3)-C(19)-F(2)	106.5(2)
F(1)-C(19)-S(1)	112.19(2)	F(3)-C(19)-S(1)	110.9(2)
F(2)-C(19)-S(1)	111.22(2)	N(2)-C(20)-C(21)	118.3(2)
N(2)-C(20)-As(2)	118.0(2)	C(21)-C(20)-As(2)	123.6(2)
C(22)-C(21)-C(20)	120.8(2)	C(22)-C(21)-H(21)	119.6

C(20)-C(21)-H(21)	119.6	C(21)-C(22)-C(23)	119.0(2)
C(21)-C(22)-H(22)	120.5	C(23)-C(22)-H(22)	120.5
C(24)-C(23)-C(22)	119.5(2)	C(24)-C(23)-H(23)	120.2
C(22)-C(23)-H(23)	120.2	N(2)-C(24)-C(23)	120.6(2)
N(2)-C(24)-H(24)	119.7	C(23)-C(24)-H(24)	119.7
N(2)-C(25)-H(25A)	109.5	N(2)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5	N(2)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5	H(25B)-C(25)-H(25C)	109.5
C(27)-C(26)-C(31)	119.7(2)	C(27)-C(26)-As(2)	124.1(2)
C(31)-C(26)-As(2)	116.1(2)	C(28)-C(27)-C(26)	119.8(2)
C(28)-C(27)-H(27)	120.1	C(26)-C(27)-H(27)	120.1
C(29)-C(28)-C(27)	120.4(2)	C(29)-C(28)-H(28)	119.8
C(27)-C(28)-H(28)	119.8	C(28)-C(29)-C(30)	119.7(2)
C(28)-C(29)-H(29)	120.2	C(30)-C(29)-H(29)	120.2
C(31)-C(30)-C(29)	120.6(2)	C(31)-C(30)-H(30)	119.7
C(29)-C(30)-H(30)	119.7	C(30)-C(31)-C(26)	119.7(2)
C(30)-C(31)-H(31)	120.2	C(26)-C(31)-H(31)	120.2
C(37)-C(32)-C(33)	118.4(2)	C(37)-C(32)-As(2)	125.8(2)
C(33)-C(32)-As(2)	115.7(2)	C(34)-C(33)-C(32)	121.0(2)
C(34)-C(33)-H(33)	119.5	C(32)-C(33)-H(33)	119.5
C(33)-C(34)-C(35)	119.8(2)	C(33)-C(34)-H(34)	120.1
C(35)-C(34)-H(34)	120.1	C(34)-C(35)-C(36)	119.7(2)
C(34)-C(35)-H(35)	120.2	C(36)-C(35)-H(35)	120.2
C(37)-C(36)-C(35)	120.2(2)	C(37)-C(36)-H(36)	119.9
C(35)-C(36)-H(36)	119.9	C(36)-C(37)-C(32)	120.8(2)
C(36)-C(37)-H(37)	119.6	C(32)-C(37)-H(37)	119.6
F(4)-C(38)-F(6)	107.7(2)	F(4)-C(38)-F(5)	107.8(2)
F(6)-C(38)-F(5)	107.2(2)	F(4)-C(38)-S(2)	111.2(2)
F(6)-C(38)-S(2)	111.6(2)	F(5)-C(38)-S(2)	111.0(2)
N(3)-C(39)-C(40)	118.5(2)	N(3)-C(39)-As(3)	118.1(2)
C(40)-C(39)-As(3)	123.4(2)	C(39)-C(40)-C(41)	120.9(2)
C(39)-C(40)-H(40)	119.6	C(41)-C(40)-H(40)	119.6
C(42)-C(41)-C(40)	118.9(2)	C(42)-C(41)-H(41)	120.5
C(40)-C(41)-H(41)	120.5	C(43)-C(42)-C(41)	119.4(2)
C(43)-C(42)-H(42)	120.3	C(41)-C(42)-H(42)	120.3
N(3)-C(43)-C(42)	120.6(2)	N(3)-C(43)-H(43)	119.7
C(42)-C(43)-H(43)	119.7	N(3)-C(44)-H(44A)	109.5
N(3)-C(44)-H(44B)	109.5	H(44A)-C(44)-H(44B)	109.5

N(3)-C(44)-H(44C)	109.5	H(44A)-C(44)-H(44C)	109.5
H(44B)-C(44)-H(44C)	109.5	C(46)-C(45)-C(50)	119.4(2)
C(46)-C(45)-As(3)	123.7(2)	C(50)-C(45)-As(3)	116.8(2)
N(4)-C(046)-H(04A)	109.5	N(4)-C(046)-H(04B)	109.5
H(04A)-C(046)-H(04B)	109.5	N(4)-C(046)-H(04C)	109.5
H(04A)-C(046)-H(04C)	109.5	H(04B)-C(046)-H(04C)	109.5
C(45)-C(46)-C(47)	119.8(2)	C(45)-C(46)-H(46)	120.1
C(47)-C(46)-H(46)	120.1	C(48)-C(47)-C(46)	120.7(2)
C(48)-C(47)-H(47)	119.6	C(46)-C(47)-H(47)	119.6
C(47)-C(48)-C(49)	119.6(2)	C(47)-C(48)-H(48)	120.2
C(49)-C(48)-H(48)	120.2	C(48)-C(49)-C(50)	120.1(2)
C(48)-C(49)-H(49)	119.9	C(50)-C(49)-H(49)	119.9
C(49)-C(50)-C(45)	120.4(2)	C(49)-C(50)-H(50)	119.8
C(45)-C(50)-H(50)	119.8	C(56)-C(51)-C(52)	119.2(2)
C(56)-C(51)-As(3)	125.49(16)	C(52)-C(51)-As(3)	115.2(2)
C(53)-C(52)-C(51)	120.6(2)	C(53)-C(52)-H(52)	119.7
C(51)-C(52)-H(52)	119.7	C(54)-C(53)-C(52)	119.8(2)
C(54)-C(53)-H(53)	120.1	C(52)-C(53)-H(53)	120.1
C(53)-C(54)-C(55)	120.0(2)	C(53)-C(54)-H(54)	120.0
C(55)-C(54)-H(54)	120.0	C(56)-C(55)-C(54)	120.1(2)
C(56)-C(55)-H(55)	119.9	C(54)-C(55)-H(55)	119.9
C(51)-C(56)-C(55)	120.14(19)	C(51)-C(56)-H(56)	119.9
C(55)-C(56)-H(56)	119.9	F(7)-C(57)-F(8)	107.2(2)
F(7)-C(57)-F(9)	107.43(16)	F(8)-C(57)-F(9)	107.5(2)
F(7)-C(57)-S(3)	111.52(14)	F(8)-C(57)-S(3)	112.3(2)
F(9)-C(57)-S(3)	110.62(15)	N(4)-C(58)-C(59)	118.3(2)
N(4)-C(58)-As(4)	118.47(14)	C(59)-C(58)-As(4)	123.2(2)
C(60)-C(59)-C(58)	120.7(2)	C(60)-C(59)-H(59)	119.6
C(58)-C(59)-H(59)	119.6	C(61)-C(60)-C(59)	119.0(2)
C(61)-C(60)-H(60)	120.5	C(59)-C(60)-H(60)	120.5
C(60)-C(61)-C(62)	119.4(2)	C(60)-C(61)-H(61)	120.3
C(62)-C(61)-H(61)	120.3	N(4)-C(62)-C(61)	120.4(2)
N(4)-C(62)-H(62)	119.8	C(61)-C(62)-H(62)	119.8
C(64)-C(63)-C(68)	119.3(2)	C(64)-C(63)-As(4)	124.2(2)
C(68)-C(63)-As(4)	116.34(15)	C(65)-C(64)-C(63)	120.0(2)
C(65)-C(64)-H(64)	120.0	C(63)-C(64)-H(64)	120.0
C(64)-C(65)-C(66)	120.5(2)	C(64)-C(65)-H(65)	119.7
C(66)-C(65)-H(65)	119.7	C(65)-C(66)-C(67)	119.7(2)

C(65)-C(66)-H(66)	120.2	C(67)-C(66)-H(66)	120.2
C(68)-C(67)-C(66)	120.3(2)	C(68)-C(67)-H(67)	119.8
C(66)-C(67)-H(67)	119.8	C(67)-C(68)-C(63)	120.1(2)
C(67)-C(68)-H(68)	120.0	C(63)-C(68)-H(68)	120.0
C(74)-C(69)-C(70)	118.7(2)	C(74)-C(69)-As(4)	125.8(2)
C(70)-C(69)-As(4)	115.36(16)	C(71)-C(70)-C(69)	120.7(2)
C(71)-C(70)-H(70)	119.7	C(69)-C(70)-H(70)	119.7
C(72)-C(71)-C(70)	120.1(2)	C(72)-C(71)-H(71)	119.9
C(70)-C(71)-H(71)	119.9	C(71)-C(72)-C(73)	119.6(2)
C(71)-C(72)-H(72)	120.2	C(73)-C(72)-H(72)	120.2
C(74)-C(73)-C(72)	120.4(2)	C(74)-C(73)-H(73)	119.8
C(72)-C(73)-H(73)	119.8	C(73)-C(74)-C(69)	120.5(2)
C(73)-C(74)-H(74)	119.7	C(69)-C(74)-H(74)	119.7
C(75B)-C(75)-F(11)	110(4)	C(75B)-C(75)-F(12)	110(4)
F(11)-C(75)-F(12)	109.34(19)	C(75B)-C(75)-F(10)	114(4)
F(11)-C(75)-F(10)	106.6(2)	F(12)-C(75)-F(10)	107.3(2)
C(75B)-C(75)-S(4B)	25(4)	F(11)-C(75)-S(4B)	122.5(3)
F(12)-C(75)-S(4B)	118.2(3)	F(10)-C(75)-S(4B)	88.9(3)
C(75B)-C(75)-S(4)	3(4)	F(11)-C(75)-S(4)	111.7(2)
F(12)-C(75)-S(4)	110.42(18)	F(10)-C(75)-S(4)	111.3(2)
S(4B)-C(75)-S(4)	22.4(3)	C(75B)-C(75)-F(10B)	62(4)
F(11)-C(75)-F(10B)	73.5(10)	F(12)-C(75)-F(10B)	77.5(10)
F(10)-C(75)-F(10B)	174.6(10)	S(4B)-C(75)-F(10B)	86.6(10)
S(4)-C(75)-F(10B)	64.1(10)	C(75)-C(75B)-S(4)	176(6)
C(75)-C(75B)-S(4B)	145(5)	S(4)-C(75B)-S(4B)	32.0(11)
C(75)-C(75B)-F(11)	51(3)	S(4)-C(75B)-F(11)	132(3)
S(4B)-C(75B)-F(11)	141(3)	C(75)-C(75B)-F(12)	50(3)
S(4)-C(75B)-F(12)	130(3)	S(4B)-C(75B)-F(12)	134(3)
F(11)-C(75B)-F(12)	84.0(18)	C(75)-C(75B)-F(10)	48(3)
S(4)-C(75B)-F(10)	129(3)	S(4B)-C(75B)-F(10)	97(2)
F(11)-C(75B)-F(10)	81.6(18)	F(12)-C(75B)-F(10)	81.9(18)
C(75)-C(75B)-F(10B)	101(4)	S(4)-C(75B)-F(10B)	83(2)
S(4B)-C(75B)-F(10B)	114(3)	F(11)-C(75B)-F(10B)	73.4(19)
F(12)-C(75B)-F(10B)	76.9(19)	F(10)-C(75B)-F(10B)	149(3)
N(5)-C(76)-C(77)	118.39(18)	N(5)-C(76)-As(5)	118.1(2)
C(77)-C(76)-As(5)	123.51(15)	C(78)-C(77)-C(76)	120.8(2)
C(78)-C(77)-H(77)	119.6	C(76)-C(77)-H(77)	119.6
C(79)-C(78)-C(77)	118.9(2)	C(79)-C(78)-H(78)	120.5

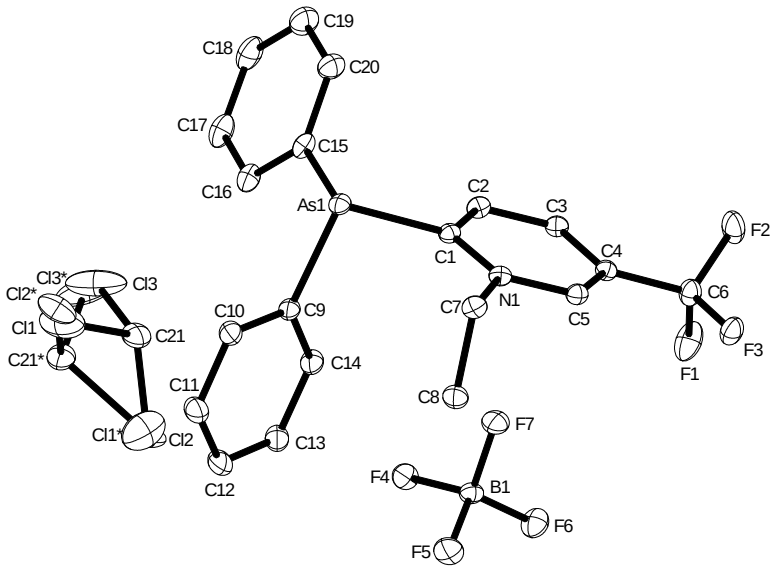
C(77)-C(78)-H(78)	120.5	C(80)-C(79)-C(78)	119.6(2)
C(80)-C(79)-H(79)	120.2	C(78)-C(79)-H(79)	120.2
N(5)-C(80)-C(79)	120.5(2)	N(5)-C(80)-H(80)	119.7
C(79)-C(80)-H(80)	119.7	N(5)-C(81)-H(81A)	109.5
N(5)-C(81)-H(81B)	109.5	H(81A)-C(81)-H(81B)	109.5
N(5)-C(81)-H(81C)	109.5	H(81A)-C(81)-H(81C)	109.5
H(81B)-C(81)-H(81C)	109.5	C(87)-C(82)-C(83)	119.7(2)
C(87)-C(82)-As(5)	115.66(15)	C(83)-C(82)-As(5)	124.7(2)
C(84)-C(83)-C(82)	120.2(2)	C(84)-C(83)-H(83)	119.9
C(82)-C(83)-H(83)	119.9	C(83)-C(84)-C(85)	120.0(2)
C(83)-C(84)-H(84)	120.0	C(85)-C(84)-H(84)	120.0
C(84)-C(85)-C(86)	120.0(2)	C(84)-C(85)-H(85)	120.0
C(86)-C(85)-H(85)	120.0	C(87)-C(86)-C(85)	120.3(2)
C(87)-C(86)-H(86)	119.9	C(85)-C(86)-H(86)	119.9
C(86)-C(87)-C(82)	119.90(19)	C(86)-C(87)-H(87)	120.1
C(82)-C(87)-H(87)	120.1	C(93)-C(88)-C(89)	118.8(2)
C(93)-C(88)-As(5)	125.98(15)	C(89)-C(88)-As(5)	115.1(2)
C(90)-C(89)-C(88)	120.8(2)	C(90)-C(89)-H(89)	119.6
C(88)-C(89)-H(89)	119.6	C(91)-C(90)-C(89)	120.0(2)
C(91)-C(90)-H(90)	120.0	C(89)-C(90)-H(90)	120.0
C(90)-C(91)-C(92)	119.8(2)	C(90)-C(91)-H(91)	120.1
C(92)-C(91)-H(91)	120.1	C(93)-C(92)-C(91)	120.0(2)
C(93)-C(92)-H(92)	120.0	C(91)-C(92)-H(92)	120.0
C(92)-C(93)-C(88)	120.56(19)	C(92)-C(93)-H(93)	119.7
C(88)-C(93)-H(93)	119.7	F(15A)-C(94)-F(14B)	68.2(3)
F(15A)-C(94)-F(13B)	112.7(7)	F(14B)-C(94)-F(13B)	111.4(5)
F(15A)-C(94)-F(13A)	114.9(7)	F(14B)-C(94)-F(13A)	126.0(5)
F(13B)-C(94)-F(13A)	14.7(7)	F(15A)-C(94)-F(14A)	105.9(3)
F(14B)-C(94)-F(14A)	38.8(3)	F(13B)-C(94)-F(14A)	88.9(5)
F(13A)-C(94)-F(14A)	101.8(5)	F(15A)-C(94)-F(15B)	36.2(2)
F(14B)-C(94)-F(15B)	104.4(4)	F(13B)-C(94)-F(15B)	99.2(7)
F(13A)-C(94)-F(15B)	93.1(7)	F(14A)-C(94)-F(15B)	141.2(3)
F(15A)-C(94)-S(5)	119.8(2)	F(14B)-C(94)-S(5)	116.0(3)
F(13B)-C(94)-S(5)	118.5(6)	F(13A)-C(94)-S(5)	107.7(5)
F(14A)-C(94)-S(5)	104.6(2)	F(15B)-C(94)-S(5)	104.5(2)
N(6)-C(95)-C(96)	118.08(19)	N(6)-C(95)-As(6)	118.6(2)
C(96)-C(95)-As(6)	123.29(16)	C(95)-C(96)-C(97)	120.9(2)
C(95)-C(96)-H(96)	119.6	C(97)-C(96)-H(96)	119.6

C(98)-C(97)-C(96)	118.9(2)	C(98)-C(97)-H(97)	120.6
C(96)-C(97)-H(97)	120.6	C(99)-C(98)-C(97)	119.5(2)
C(99)-C(98)-H(98)	120.3	C(97)-C(98)-H(98)	120.3
N(6)-C(99)-C(98)	120.8(2)	N(6)-C(99)-H(99)	119.6
C(98)-C(99)-H(99)	119.6	N(6)-C(100)-H(10A)	109.5
N(6)-C(100)-H(10B)	109.5	H(10A)-C(100)-H(10B)	109.5
N(6)-C(100)-H(10C)	109.5	H(10A)-C(100)-H(10C)	109.5
H(10B)-C(100)-H(10C)	109.5	C(106)-C(101)-C(102)	119.4(2)
C(106)-C(101)-As(6)	116.22(16)	C(102)-C(101)-As(6)	124.4(2)
C(101)-C(102)-C(103)	119.8(2)	C(101)-C(102)-H(102)	120.1
C(103)-C(102)-H(102)	120.1	C(104)-C(103)-C(102)	120.5(2)
C(104)-C(103)-H(103)	119.7	C(102)-C(103)-H(103)	119.7
C(103)-C(104)-C(105)	120.0(2)	C(103)-C(104)-H(104)	120.0
C(105)-C(104)-H(104)	120.0	C(104)-C(105)-C(106)	119.7(2)
C(104)-C(105)-H(105)	120.2	C(106)-C(105)-H(105)	120.2
C(101)-C(106)-C(105)	120.6(2)	C(101)-C(106)-H(106)	119.7
C(105)-C(106)-H(106)	119.7	C(112)-C(107)-C(108)	119.1(2)
C(112)-C(107)-As(6)	125.82(15)	C(108)-C(107)-As(6)	115.1(2)
C(109)-C(108)-C(107)	120.4(2)	C(109)-C(108)-H(108)	119.8
C(107)-C(108)-H(108)	119.8	C(110)-C(109)-C(108)	120.0(2)
C(110)-C(109)-H(109)	120.0	C(108)-C(109)-H(109)	120.0
C(109)-C(110)-C(111)	120.0(2)	C(109)-C(110)-H(110)	120.0
C(111)-C(110)-H(110)	120.0	C(110)-C(111)-C(112)	120.2(2)
C(110)-C(111)-H(111)	119.9	C(112)-C(111)-H(111)	119.9
C(107)-C(112)-C(111)	120.29(19)	C(107)-C(112)-H(112)	119.9
C(111)-C(112)-H(112)	119.9	F(16)-C(113)-F(18)	107.8(2)
F(16)-C(113)-F(17)	107.45(19)	F(18)-C(113)-F(17)	106.9(2)
F(16)-C(113)-S(6)	111.97(16)	F(18)-C(113)-S(6)	111.4(2)
F(17)-C(113)-S(6)	111.05(17)	C(5)-N(1)-C(1)	121.8(2)
C(5)-N(1)-C(6)	117.62(18)	C(1)-N(1)-C(6)	120.5(2)
C(24)-N(2)-C(20)	121.82(18)	C(24)-N(2)-C(25)	118.3(2)
C(20)-N(2)-C(25)	119.88(18)	C(43)-N(3)-C(39)	121.7(2)
C(43)-N(3)-C(44)	118.57(19)	C(39)-N(3)-C(44)	119.8(2)
C(62)-N(4)-C(58)	122.06(18)	C(62)-N(4)-C(046)	117.8(2)
C(58)-N(4)-C(046)	120.16(18)	C(80)-N(5)-C(76)	121.6(2)
C(80)-N(5)-C(81)	118.12(18)	C(76)-N(5)-C(81)	120.2(2)
C(99)-N(6)-C(95)	121.85(18)	C(99)-N(6)-C(100)	118.2(2)
C(95)-N(6)-C(100)	119.94(18)	F(10B)-O(10)-S(4)	91.4(14)

F(10B)-O(10)-S(4B)	91.2(14)	S(4)-O(10)-S(4B)	0.2(2)
S(4B)-O(10B)-F(10)	92.7(15)	S(4B)-O(10B)-S(4)	5.8(4)
F(10)-O(10B)-S(4)	87.0(12)	S(4B)-O(11)-S(4)	29.6(4)
S(4B)-O(12)-S(4)	29.1(4)	O(13B)-O(13A)-S(5)	108.0(13)
O(13A)-O(13B)-S(5)	52.1(10)	O(14B)-O(14A)-S(5)	63.7(3)
O(14A)-O(14B)-S(5)	69.4(3)	O(14A)-O(14B)-O(15A)	116.6(4)
S(5)-O(14B)-O(15A)	49.9(2)	O(15B)-O(15A)-S(5)	87.1(4)
O(15B)-O(15A)-O(14B)	140.2(5)	S(5)-O(15A)-O(14B)	57.7(2)
O(15A)-O(15B)-S(5)	58.0(4)	C(75)-F(10)-O(10B)	95.7(10)
C(75)-F(10)-C(75B)	18.6(13)	O(10B)-F(10)-C(75B)	77.1(16)
O(10)-F(10B)-C(75B)	85(2)	O(10)-F(10B)-C(75)	102.8(18)
C(75B)-F(10B)-C(75)	17.3(13)	O(10)-F(10B)-S(4)	46.7(10)
C(75B)-F(10B)-S(4)	38.8(15)	C(75)-F(10B)-S(4)	56.1(9)
C(75)-F(11)-C(75B)	19.7(13)	C(75)-F(12)-C(75B)	19.5(14)
F(14B)-F(14A)-C(94)	60.2(3)	F(14A)-F(14B)-C(94)	81.0(4)
F(14A)-F(14B)-F(15A)	134.6(5)	C(94)-F(14B)-F(15A)	55.7(3)
F(15B)-F(15A)-C(94)	84.1(4)	F(15B)-F(15A)-F(14B)	140.2(5)
C(94)-F(15A)-F(14B)	56.1(2)	F(15A)-F(15B)-C(94)	59.7(3)
O(2)-S(1)-O(1)	116.02(12)	O(2)-S(1)-O(3)	114.2(1)
O(1)-S(1)-O(3)	115.05(12)	O(2)-S(1)-C(19)	103.0(1)
O(1)-S(1)-C(19)	102.95(11)	O(3)-S(1)-C(19)	103.0(1)
O(6)-S(2)-O(4)	115.87(13)	O(6)-S(2)-O(5)	113.8(2)
O(4)-S(2)-O(5)	115.54(12)	O(6)-S(2)-C(38)	102.6(2)
O(4)-S(2)-C(38)	102.92(11)	O(5)-S(2)-C(38)	103.5(1)
O(8)-S(3)-O(7)	115.30(11)	O(8)-S(3)-O(9)	114.7(1)
O(7)-S(3)-O(9)	115.05(11)	O(8)-S(3)-C(57)	102.3(1)
O(7)-S(3)-C(57)	103.26(10)	O(9)-S(3)-C(57)	103.8(1)
S(4B)-S(4)-C(75B)	79.0(18)	S(4B)-S(4)-O(11)	64.5(6)
C(75B)-S(4)-O(11)	104.5(17)	S(4B)-S(4)-O(10)	179.3(6)
C(75B)-S(4)-O(10)	100.6(17)	O(11)-S(4)-O(10)	115.1(2)
S(4B)-S(4)-O(12)	66.0(6)	C(75B)-S(4)-O(12)	103.7(18)
O(11)-S(4)-O(12)	115.60(11)	O(10)-S(4)-O(12)	114.7(2)
S(4B)-S(4)-C(75)	77.9(6)	C(75B)-S(4)-C(75)	1.2(18)
O(11)-S(4)-C(75)	103.57(11)	O(10)-S(4)-C(75)	101.6(2)
O(12)-S(4)-C(75)	103.61(11)	S(4B)-S(4)-F(10B)	137.6(11)
C(75B)-S(4)-F(10B)	58.7(19)	O(11)-S(4)-F(10B)	121.8(9)
O(10)-S(4)-F(10B)	41.9(9)	O(12)-S(4)-F(10B)	122.5(9)
C(75)-S(4)-F(10B)	59.8(9)	S(4B)-S(4)-O(10B)	12.1(9)

C(75B)-S(4)-O(10B)	67.0(18)	O(11)-S(4)-O(10B)	71.2(8)
O(10)-S(4)-O(10B)	167.5(7)	O(12)-S(4)-O(10B)	68.9(8)
C(75)-S(4)-O(10B)	65.9(7)	F(10B)-S(4)-O(10B)	125.7(12)
S(4)-S(4B)-O(11)	85.9(8)	S(4)-S(4B)-C(75B)	69.1(18)
O(11)-S(4B)-C(75B)	108.9(18)	S(4)-S(4B)-O(12)	84.9(7)
O(11)-S(4B)-O(12)	136.5(6)	C(75B)-S(4B)-O(12)	107.2(17)
S(4)-S(4B)-O(10B)	162.1(14)	O(11)-S(4B)-O(10B)	103.1(13)
C(75B)-S(4B)-O(10B)	93(2)	O(12)-S(4B)-O(10B)	98.3(12)
S(4)-S(4B)-C(75)	79.7(6)	O(11)-S(4B)-C(75)	110.4(5)
C(75B)-S(4B)-C(75)	10.6(17)	O(12)-S(4B)-C(75)	109.6(5)
O(10B)-S(4B)-C(75)	82.7(11)	S(4)-S(4B)-O(10)	0.5(4)
O(11)-S(4B)-O(10)	85.7(5)	C(75B)-S(4B)-O(10)	68.8(17)
O(12)-S(4B)-O(10)	85.4(4)	O(10B)-S(4B)-O(10)	161.8(12)
C(75)-S(4B)-O(10)	79.3(3)	O(13A)-S(5)-O(15A)	127.5(3)
O(13A)-S(5)-O(14B)	126.4(4)	O(15A)-S(5)-O(14B)	72.4(3)
O(13A)-S(5)-O(14A)	86.1(3)	O(15A)-S(5)-O(14A)	116.7(3)
O(14B)-S(5)-O(14A)	46.9(3)	O(13A)-S(5)-O(13B)	19.9(4)
O(15A)-S(5)-O(13B)	118.4(3)	O(14B)-S(5)-O(13B)	145.3(3)
O(14A)-S(5)-O(13B)	105.7(2)	O(13A)-S(5)-O(15B)	113.3(3)
O(15A)-S(5)-O(15B)	34.9(2)	O(14B)-S(5)-O(15B)	105.3(3)
O(14A)-S(5)-O(15B)	151.4(3)	O(13B)-S(5)-O(15B)	96.1(3)
O(13A)-S(5)-C(94)	109.4(3)	O(15A)-S(5)-C(94)	112.6(2)
O(14B)-S(5)-C(94)	102.58(17)	O(14A)-S(5)-C(94)	98.27(16)
O(13B)-S(5)-C(94)	102.5(2)	O(15B)-S(5)-C(94)	94.70(19)
O(16)-S(6)-O(17)	115.19(12)	O(16)-S(6)-O(18)	116.1(2)
O(17)-S(6)-O(18)	114.35(11)	O(16)-S(6)-C(113)	103.1(1)
O(17)-S(6)-C(113)	102.58(11)	O(18)-S(6)-C(113)	102.8(1)
C(7)-As(1)-C(13)	98.84(9)	C(7)-As(1)-C(1)	96.68(8)
C(13)-As(1)-C(1)	97.12(8)	C(32)-As(2)-C(26)	100.17(9)
C(32)-As(2)-C(20)	97.02(9)	C(26)-As(2)-C(20)	96.43(8)
C(45)-As(3)-C(51)	99.92(9)	C(45)-As(3)-C(39)	97.40(9)
C(51)-As(3)-C(39)	97.04(9)	C(63)-As(4)-C(69)	99.50(9)
C(63)-As(4)-C(58)	97.14(8)	C(69)-As(4)-C(58)	97.10(9)
C(82)-As(5)-C(88)	99.79(8)	C(82)-As(5)-C(76)	95.76(8)
C(88)-As(5)-C(76)	97.75(8)	C(107)-As(6)-C(101)	100.35(9)
C(107)-As(6)-C(95)	97.94(9)	C(101)-As(6)-C(95)	95.64(8)

Symmetry transformations used to generate equivalent atoms:



Fully labeled solid-state structure of **13**.

Crystal data and structure refinement for 13.

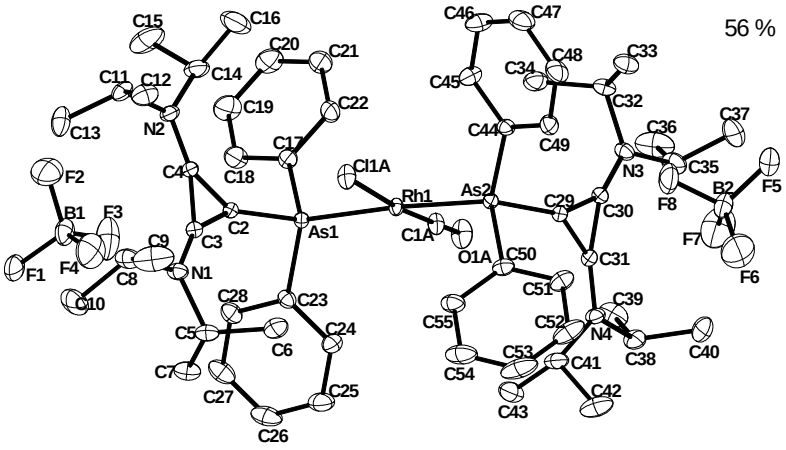
CCDC	1408075	
Empirical formula	$C_{20}\,H_{18}\,As\,B\,F_7\,N$, ½ (C H Cl_3)	
Color	colourless	
Formula weight	550.77 g·mol^{-1}	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	C 2/c, (no. 15)	
Unit cell dimensions	a = 28.5487(6) Å	α= 90°.
	b = 9.8280(13) Å	β= 104.618(4)°.
	c = 16.3361(7) Å	γ = 90°.
Volume	4435.2(6) Å^3	
Z	8	
Density (calculated)	1.650 Mg·m^{-3}	
Absorption coefficient	1.781 mm^{-1}	
F(000)	2200 e	
Crystal size	0.14 x 0.09 x 0.04 mm^3	
θ range for data collection	2.626 to 33.180°.	
Index ranges	-43 ≤ h ≤ 43, -15≤ k ≤ 15, -24≤ l ≤ 25	
Reflections collected	51738	
Independent reflections	8453 [R_{int} = 0.0366]	
Reflections with I > 2σ(I)	7257	
Completeness to θ = 25.242°	99.6 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.94037 and 0.80494	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8453 / 6 / 308	
Goodness-of-fit on F^2	1.044	
Final R indices [I > 2σ(I)]	R1 = 0.0312	wR2 = 0.0772
R indices (all data)	R1 = 0.0400	wR2 = 0.0828
Extinction coefficient	0	
Largest diff. peak and hole	0.632 and -0.703 e·Å^{-3}	

Selected bond lengths [Å] and angles [°] for 13.

As(1)-C(1)	1.9865(13)	As(1)-C(9)	1.9524(13)
As(1)-C(15)	1.9475(15)	C(1)-C(2)	1.3921(18)
C(1)-N(1)	1.3612(16)	C(2)-C(3)	1.3868(18)
C(3)-C(4)	1.3890(18)	C(4)-C(5)	1.3759(18)
C(4)-C(6)	1.4955(19)	C(5)-N(1)	1.3506(17)
C(6)-F(1)	1.3390(19)	C(6)-F(2)	1.3396(18)
C(6)-F(3)	1.3349(16)	C(7)-C(8)	1.522(2)
C(7)-N(1)	1.4940(17)	C(9)-C(10)	1.397(2)
C(9)-C(14)	1.3986(18)	C(10)-C(11)	1.395(2)
C(11)-C(12)	1.384(2)	C(12)-C(13)	1.396(3)
C(13)-C(14)	1.389(2)	C(15)-C(16)	1.389(2)
C(15)-C(20)	1.396(2)	C(16)-C(17)	1.398(2)
C(17)-C(18)	1.375(3)	C(18)-C(19)	1.380(3)
C(19)-C(20)	1.395(2)	C(21)-Cl(1)	1.821(5)
C(21)-Cl(2)	1.714(4)	C(21)-Cl(3)	1.774(4)
B(1)-F(4)	1.3952(17)	B(1)-F(5)	1.3965(17)
B(1)-F(6)	1.3892(19)	B(1)-F(7)	1.3912(17)
C(9)-As(1)-C(1)	97.12(5)	C(15)-As(1)-C(1)	97.38(5)
C(15)-As(1)-C(9)	101.16(6)	C(2)-C(1)-As(1)	122.31(9)
N(1)-C(1)-As(1)	119.23(9)	N(1)-C(1)-C(2)	118.35(12)
C(3)-C(2)-C(1)	120.85(12)	C(2)-C(3)-C(4)	118.66(12)
C(3)-C(4)-C(6)	119.59(12)	C(5)-C(4)-C(3)	119.79(12)
C(5)-C(4)-C(6)	120.61(12)	N(1)-C(5)-C(4)	120.40(12)
F(1)-C(6)-C(4)	111.05(12)	F(1)-C(6)-F(2)	106.92(13)
F(2)-C(6)-C(4)	111.60(13)	F(3)-C(6)-C(4)	112.83(11)
F(3)-C(6)-F(1)	106.78(13)	F(3)-C(6)-F(2)	107.34(12)
N(1)-C(7)-C(8)	111.08(11)	C(10)-C(9)-As(1)	116.78(10)
C(10)-C(9)-C(14)	119.61(13)	C(14)-C(9)-As(1)	123.53(11)
C(11)-C(10)-C(9)	120.41(14)	C(12)-C(11)-C(10)	119.64(16)
C(11)-C(12)-C(13)	120.26(15)	C(14)-C(13)-C(12)	120.30(14)
C(13)-C(14)-C(9)	119.74(14)	C(16)-C(15)-As(1)	122.74(12)
C(16)-C(15)-C(20)	119.88(14)	C(20)-C(15)-As(1)	117.22(12)
C(15)-C(16)-C(17)	119.74(16)	C(18)-C(17)-C(16)	120.40(17)
C(17)-C(18)-C(19)	119.94(17)	C(18)-C(19)-C(20)	120.71(18)
C(19)-C(20)-C(15)	119.30(17)	C(1)-N(1)-C(7)	122.46(11)

C(5)-N(1)-C(1)	121.93(11)	C(5)-N(1)-C(7)	115.60(11)
Cl(2)-C(21)-Cl(1)	108.6(2)	Cl(2)-C(21)-Cl(3)	112.5(3)
Cl(3)-C(21)-Cl(1)	105.7(3)	F(4)-B(1)-F(5)	109.06(12)
F(6)-B(1)-F(4)	109.30(12)	F(6)-B(1)-F(5)	109.46(12)
F(6)-B(1)-F(7)	109.65(12)	F(7)-B(1)-F(4)	109.12(12)
F(7)-B(1)-F(5)	110.23(12)		

Symmetry transformations used to generate equivalent atoms:



Fully labeled solid-state structure of **14**.

Crystal data and structure refinement for 14.

CCDC	1408073	
Empirical formula	C_{55} H_{76} As_2 B_2 Cl F_8 N_4 O Rh	
Color	colourless	
Formula weight	1271.01 g·mol^{-1}	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	ORTHORHOMBIC	
Space group	p 21 21 21, (no. 19)	
Unit cell dimensions	a = 14.384(6) Å	α= 90°.
	b = 15.902(7) Å	β= 90°.
	c = 26.833(12) Å	γ = 90°.
Volume	6138(5) Å^3	
Z	4	
Density (calculated)	1.375 Mg·m^{-3}	
Absorption coefficient	1.455 mm^{-1}	
F(000)	2608 e	
Crystal size	0.30 x 0.29 x 0.16 mm^3	
θ range for data collection	1.489 to 35.659°.	
Index ranges	-23 ≤ h ≤ 23, -26≤ k ≤ 26, -44 ≤ l ≤ 43	
Reflections collected	192484	
Independent reflections	28221 [R_{int} = 0.0368]	
Reflections with I>2σ(I)	25698	
Completeness to θ = 25.242°	99.0 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.82864 and 0.66219	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	28221 / 0 / 712	
Goodness-of-fit on F^2	1.099	
Final R indices [I>2σ(I)]	R_1 = 0.0263	wR^2 = 0.0630
R indices (all data)	R_1 = 0.0330	wR^2 = 0.0687
Absolute structure parameter	0.401(4)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.779 and -0.992 e·Å^{-3}	

Bond lengths [Å] and angles [°] for 14.

C(1A)-O(1A)	1.154(12)	C(1A)-Rh(1)	1.802(7)
C(1B)-O(1B)	1.135(15)	C(1B)-Rh(1)	1.788(9)
C(2)-C(3)	1.379(3)	C(2)-C(4)	1.384(2)
C(2)-As(1)	1.9218(18)	C(3)-C(4)	1.415(3)
C(3)-N(1)	1.313(2)	C(4)-N(2)	1.306(2)
C(5)-H(5)	1.0000	C(5)-C(6)	1.518(3)
C(5)-C(7)	1.516(3)	C(5)-N(1)	1.493(3)
C(6)-H(6A)	0.9800	C(6)-H(6B)	0.9800
C(6)-H(6C)	0.9800	C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800	C(7)-H(7C)	0.9800
C(8)-H(8)	1.0000	C(8)-C(9)	1.529(4)
C(8)-C(10)	1.519(4)	C(8)-N(1)	1.485(3)
C(9)-H(9A)	0.9800	C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800	C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800	C(10)-H(10C)	0.9800
C(11)-H(11)	1.0000	C(11)-C(12)	1.521(3)
C(11)-C(13)	1.526(4)	C(11)-N(2)	1.487(3)
C(12)-H(12A)	0.9800	C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800	C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800	C(13)-H(13C)	0.9800
C(14)-H(14)	1.0000	C(14)-C(15)	1.526(4)
C(14)-C(16)	1.517(4)	C(14)-N(2)	1.492(3)
C(15)-H(15A)	0.9800	C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800	C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800	C(16)-H(16C)	0.9800
C(17)-C(18)	1.395(3)	C(17)-C(22)	1.393(3)
C(17)-As(1)	1.933(2)	C(18)-H(18)	0.9500
C(18)-C(19)	1.399(3)	C(19)-H(19)	0.9500
C(19)-C(20)	1.380(4)	C(20)-H(20)	0.9500
C(20)-C(21)	1.379(4)	C(21)-H(21)	0.9500
C(21)-C(22)	1.394(3)	C(22)-H(22)	0.9500
C(23)-C(24)	1.394(3)	C(23)-C(28)	1.394(3)
C(23)-As(1)	1.930(2)	C(24)-H(24)	0.9500
C(24)-C(25)	1.394(3)	C(25)-H(25)	0.9500
C(25)-C(26)	1.382(4)	C(26)-H(26)	0.9500
C(26)-C(27)	1.386(4)	C(27)-H(27)	0.9500

C(27)-C(28)	1.394(3)	C(28)-H(28)	0.9500
C(29)-C(30)	1.384(3)	C(29)-C(31)	1.385(2)
C(29)-As(2)	1.9196(18)	C(30)-C(31)	1.415(3)
C(30)-N(3)	1.307(2)	C(31)-N(4)	1.307(2)
C(32)-H(32)	1.0000	C(32)-C(33)	1.524(3)
C(32)-C(34)	1.523(3)	C(32)-N(3)	1.494(3)
C(33)-H(33A)	0.9800	C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800	C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800	C(34)-H(34C)	0.9800
C(35)-H(35)	1.0000	C(35)-C(36)	1.520(4)
C(35)-C(37)	1.529(4)	C(35)-N(3)	1.481(3)
C(36)-H(36A)	0.9800	C(36)-H(36B)	0.9800
C(36)-H(36C)	0.9800	C(37)-H(37A)	0.9800
C(37)-H(37B)	0.9800	C(37)-H(37C)	0.9800
C(38)-H(38)	1.0000	C(38)-C(39)	1.525(4)
C(38)-C(40)	1.526(4)	C(38)-N(4)	1.490(3)
C(39)-H(39A)	0.9800	C(39)-H(39B)	0.9800
C(39)-H(39C)	0.9800	C(40)-H(40A)	0.9800
C(40)-H(40B)	0.9800	C(40)-H(40C)	0.9800
C(41)-H(41)	1.0000	C(41)-C(42)	1.526(3)
C(41)-C(43)	1.533(4)	C(41)-N(4)	1.494(3)
C(42)-H(42A)	0.9800	C(42)-H(42B)	0.9800
C(42)-H(42C)	0.9800	C(43)-H(43A)	0.9800
C(43)-H(43B)	0.9800	C(43)-H(43C)	0.9800
C(44)-C(45)	1.397(3)	C(44)-C(49)	1.396(3)
C(44)-As(2)	1.936(2)	C(45)-H(45)	0.9500
C(45)-C(46)	1.400(3)	C(46)-H(46)	0.9500
C(46)-C(47)	1.385(4)	C(47)-H(47)	0.9500
C(47)-C(48)	1.383(4)	C(48)-H(48)	0.9500
C(48)-C(49)	1.391(3)	C(49)-H(49)	0.9500
C(50)-C(51)	1.399(3)	C(50)-C(55)	1.396(3)
C(50)-As(2)	1.931(2)	C(51)-H(51)	0.9500
C(51)-C(52)	1.400(3)	C(52)-H(52)	0.9500
C(52)-C(53)	1.381(5)	C(53)-H(53)	0.9500
C(53)-C(54)	1.387(5)	C(54)-H(54)	0.9500
C(54)-C(55)	1.398(3)	C(55)-H(55)	0.9500
Cl(1A)-Rh(1)	2.3602(17)	Cl(1B)-Rh(1)	2.372(2)
As(1)-Rh(1)	2.3915(9)	As(2)-Rh(1)	2.3942(8)

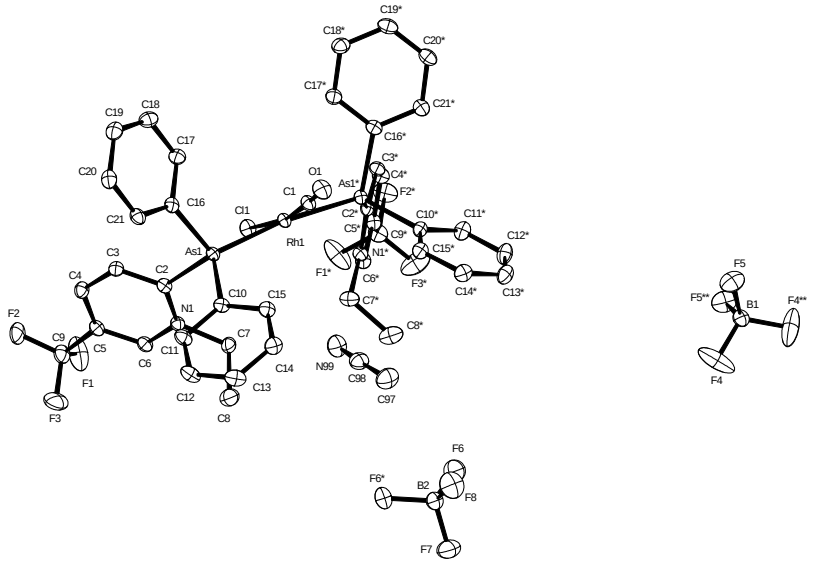
B(1)-F(1)	1.386(3)	B(1)-F(2)	1.386(3)
B(1)-F(3)	1.397(3)	B(1)-F(4)	1.393(3)
B(2)-F(5)	1.392(3)	B(2)-F(6)	1.369(3)
B(2)-F(7)	1.373(3)	B(2)-F(8)	1.390(3)

O(1A)-C(1A)-Rh(1)	179.1(5)	O(1B)-C(1B)-Rh(1)	178.9(5)
C(3)-C(2)-C(4)	61.62(13)	C(3)-C(2)-As(1)	150.35(14)
C(4)-C(2)-As(1)	145.67(14)	C(2)-C(3)-C(4)	59.35(13)
N(1)-C(3)-C(2)	151.06(18)	N(1)-C(3)-C(4)	149.48(18)
C(2)-C(4)-C(3)	59.03(12)	N(2)-C(4)-C(2)	146.71(18)
N(2)-C(4)-C(3)	154.14(18)	C(6)-C(5)-H(5)	106.8
C(7)-C(5)-H(5)	106.8	C(7)-C(5)-C(6)	113.4(2)
N(1)-C(5)-H(5)	106.8	N(1)-C(5)-C(6)	111.31(18)
N(1)-C(5)-C(7)	111.36(18)	C(5)-C(6)-H(6A)	109.5
C(5)-C(6)-H(6B)	109.5	C(5)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6B)	109.5	H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5	C(5)-C(7)-H(7A)	109.5
C(5)-C(7)-H(7B)	109.5	C(5)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7B)	109.5	H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5	C(9)-C(8)-H(8)	107.2
C(10)-C(8)-H(8)	107.2	C(10)-C(8)-C(9)	113.3(3)
N(1)-C(8)-H(8)	107.2	N(1)-C(8)-C(9)	110.2(2)
N(1)-C(8)-C(10)	111.3(2)	C(8)-C(9)-H(9A)	109.5
C(8)-C(9)-H(9B)	109.5	C(8)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9B)	109.5	H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5	C(8)-C(10)-H(10A)	109.5
C(8)-C(10)-H(10B)	109.5	C(8)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10B)	109.5	H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5	C(12)-C(11)-H(11)	106.1
C(12)-C(11)-C(13)	116.0(2)	C(13)-C(11)-H(11)	106.1
N(2)-C(11)-H(11)	106.1	N(2)-C(11)-C(12)	110.94(17)
N(2)-C(11)-C(13)	110.75(17)	C(11)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12B)	109.5	C(11)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12B)	109.5	H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5	C(11)-C(13)-H(13A)	109.5
C(11)-C(13)-H(13B)	109.5	C(11)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13B)	109.5	H(13A)-C(13)-H(13C)	109.5

H(13B)-C(13)-H(13C)	109.5	C(15)-C(14)-H(14)	107.3
C(16)-C(14)-H(14)	107.3	C(16)-C(14)-C(15)	113.4(2)
N(2)-C(14)-H(14)	107.3	N(2)-C(14)-C(15)	110.7(2)
N(2)-C(14)-C(16)	110.5(2)	C(14)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5	C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15B)	109.5	H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5	C(14)-C(16)-H(16A)	109.5
C(14)-C(16)-H(16B)	109.5	C(14)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16B)	109.5	H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5	C(18)-C(17)-As(1)	123.36(17)
C(22)-C(17)-C(18)	119.93(19)	C(22)-C(17)-As(1)	116.46(16)
C(17)-C(18)-H(18)	120.4	C(17)-C(18)-C(19)	119.2(2)
C(19)-C(18)-H(18)	120.4	C(18)-C(19)-H(19)	119.8
C(20)-C(19)-C(18)	120.4(2)	C(20)-C(19)-H(19)	119.8
C(19)-C(20)-H(20)	119.7	C(21)-C(20)-C(19)	120.5(2)
C(21)-C(20)-H(20)	119.7	C(20)-C(21)-H(21)	120.1
C(20)-C(21)-C(22)	119.8(2)	C(22)-C(21)-H(21)	120.1
C(17)-C(22)-C(21)	120.1(2)	C(17)-C(22)-H(22)	120.0
C(21)-C(22)-H(22)	120.0	C(24)-C(23)-C(28)	120.48(19)
C(24)-C(23)-As(1)	118.11(15)	C(28)-C(23)-As(1)	121.30(15)
C(23)-C(24)-H(24)	120.4	C(23)-C(24)-C(25)	119.2(2)
C(25)-C(24)-H(24)	120.4	C(24)-C(25)-H(25)	119.7
C(26)-C(25)-C(24)	120.5(2)	C(26)-C(25)-H(25)	119.7
C(25)-C(26)-H(26)	119.9	C(25)-C(26)-C(27)	120.2(2)
C(27)-C(26)-H(26)	119.9	C(26)-C(27)-H(27)	119.9
C(26)-C(27)-C(28)	120.2(2)	C(28)-C(27)-H(27)	119.9
C(23)-C(28)-H(28)	120.3	C(27)-C(28)-C(23)	119.5(2)
C(27)-C(28)-H(28)	120.3	C(30)-C(29)-C(31)	61.47(13)
C(30)-C(29)-As(2)	152.39(14)	C(31)-C(29)-As(2)	142.56(15)
C(29)-C(30)-C(31)	59.31(13)	N(3)-C(30)-C(29)	148.89(18)
N(3)-C(30)-C(31)	151.50(18)	C(29)-C(31)-C(30)	59.21(13)
N(4)-C(31)-C(29)	147.28(18)	N(4)-C(31)-C(30)	153.24(17)
C(33)-C(32)-H(32)	107.1	C(34)-C(32)-H(32)	107.1
C(34)-C(32)-C(33)	113.20(19)	N(3)-C(32)-H(32)	107.1
N(3)-C(32)-C(33)	111.32(17)	N(3)-C(32)-C(34)	110.63(18)
C(32)-C(33)-H(33A)	109.5	C(32)-C(33)-H(33B)	109.5
C(32)-C(33)-H(33C)	109.5	H(33A)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33C)	109.5	H(33B)-C(33)-H(33C)	109.5

C(32)-C(34)-H(34A)	109.5	C(32)-C(34)-H(34B)	109.5
C(32)-C(34)-H(34C)	109.5	H(34A)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34C)	109.5	H(34B)-C(34)-H(34C)	109.5
C(36)-C(35)-H(35)	107.5	C(36)-C(35)-C(37)	112.6(2)
C(37)-C(35)-H(35)	107.5	N(3)-C(35)-H(35)	107.5
N(3)-C(35)-C(36)	110.7(2)	N(3)-C(35)-C(37)	110.8(2)
C(35)-C(36)-H(36A)	109.5	C(35)-C(36)-H(36B)	109.5
C(35)-C(36)-H(36C)	109.5	H(36A)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36C)	109.5	H(36B)-C(36)-H(36C)	109.5
C(35)-C(37)-H(37A)	109.5	C(35)-C(37)-H(37B)	109.5
C(35)-C(37)-H(37C)	109.5	H(37A)-C(37)-H(37B)	109.5
H(37A)-C(37)-H(37C)	109.5	H(37B)-C(37)-H(37C)	109.5
C(39)-C(38)-H(38)	106.4	C(39)-C(38)-C(40)	115.3(2)
C(40)-C(38)-H(38)	106.4	N(4)-C(38)-H(38)	106.4
N(4)-C(38)-C(39)	110.60(18)	N(4)-C(38)-C(40)	111.24(19)
C(38)-C(39)-H(39A)	109.5	C(38)-C(39)-H(39B)	109.5
C(38)-C(39)-H(39C)	109.5	H(39A)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39C)	109.5	H(39B)-C(39)-H(39C)	109.5
C(38)-C(40)-H(40A)	109.5	C(38)-C(40)-H(40B)	109.5
C(38)-C(40)-H(40C)	109.5	H(40A)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40C)	109.5	H(40B)-C(40)-H(40C)	109.5
C(42)-C(41)-H(41)	107.6	C(42)-C(41)-C(43)	112.2(2)
C(43)-C(41)-H(41)	107.6	N(4)-C(41)-H(41)	107.6
N(4)-C(41)-C(42)	110.4(2)	N(4)-C(41)-C(43)	111.07(19)
C(41)-C(42)-H(42A)	109.5	C(41)-C(42)-H(42B)	109.5
C(41)-C(42)-H(42C)	109.5	H(42A)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42C)	109.5	H(42B)-C(42)-H(42C)	109.5
C(41)-C(43)-H(43A)	109.5	C(41)-C(43)-H(43B)	109.5
C(41)-C(43)-H(43C)	109.5	H(43A)-C(43)-H(43B)	109.5
H(43A)-C(43)-H(43C)	109.5	H(43B)-C(43)-H(43C)	109.5
C(45)-C(44)-As(2)	117.87(15)	C(49)-C(44)-C(45)	120.01(18)
C(49)-C(44)-As(2)	122.06(14)	C(44)-C(45)-H(45)	120.4
C(44)-C(45)-C(46)	119.2(2)	C(46)-C(45)-H(45)	120.4
C(45)-C(46)-H(46)	119.7	C(47)-C(46)-C(45)	120.6(2)
C(47)-C(46)-H(46)	119.7	C(46)-C(47)-H(47)	120.1
C(48)-C(47)-C(46)	119.9(2)	C(48)-C(47)-H(47)	120.1
C(47)-C(48)-H(48)	119.8	C(47)-C(48)-C(49)	120.5(2)
C(49)-C(48)-H(48)	119.8	C(44)-C(49)-H(49)	120.1

C(48)-C(49)-C(44)	119.8(2)	C(48)-C(49)-H(49)	120.1
C(51)-C(50)-As(2)	121.11(16)	C(55)-C(50)-C(51)	121.09(19)
C(55)-C(50)-As(2)	117.67(16)	C(50)-C(51)-H(51)	120.7
C(50)-C(51)-C(52)	118.5(2)	C(52)-C(51)-H(51)	120.7
C(51)-C(52)-H(52)	119.7	C(53)-C(52)-C(51)	120.6(3)
C(53)-C(52)-H(52)	119.7	C(52)-C(53)-H(53)	119.7
C(52)-C(53)-C(54)	120.6(2)	C(54)-C(53)-H(53)	119.7
C(53)-C(54)-H(54)	120.0	C(53)-C(54)-C(55)	119.9(3)
C(55)-C(54)-H(54)	120.0	C(50)-C(55)-C(54)	119.2(2)
C(50)-C(55)-H(55)	120.4	C(54)-C(55)-H(55)	120.4
C(3)-N(1)-C(5)	121.37(17)	C(3)-N(1)-C(8)	120.19(17)
C(8)-N(1)-C(5)	118.43(17)	C(4)-N(2)-C(11)	123.70(16)
C(4)-N(2)-C(14)	118.03(16)	C(11)-N(2)-C(14)	118.24(16)
C(30)-N(3)-C(32)	119.57(16)	C(30)-N(3)-C(35)	121.17(18)
C(35)-N(3)-C(32)	119.20(17)	C(31)-N(4)-C(38)	123.23(17)
C(31)-N(4)-C(41)	118.87(16)	C(38)-N(4)-C(41)	117.61(16)
C(2)-As(1)-C(17)	101.83(8)	C(2)-As(1)-C(23)	101.65(8)
C(2)-As(1)-Rh(1)	113.98(6)	C(17)-As(1)-Rh(1)	112.79(7)
C(23)-As(1)-C(17)	108.60(9)	C(23)-As(1)-Rh(1)	116.49(7)
C(29)-As(2)-C(44)	107.37(8)	C(29)-As(2)-C(50)	99.04(8)
C(29)-As(2)-Rh(1)	111.98(6)	C(44)-As(2)-Rh(1)	117.15(7)
C(50)-As(2)-C(44)	105.85(8)	C(50)-As(2)-Rh(1)	113.72(7)
C(1A)-Rh(1)-Cl(1A)	175.49(15)	C(1A)-Rh(1)-As(1)	89.32(14)
C(1A)-Rh(1)-As(2)	90.84(13)	C(1B)-Rh(1)-Cl(1B)	175.54(18)
C(1B)-Rh(1)-As(1)	89.20(17)	C(1B)-Rh(1)-As(2)	90.87(17)
Cl(1A)-Rh(1)-As(1)	92.30(3)	Cl(1A)-Rh(1)-As(2)	87.82(4)
Cl(1B)-Rh(1)-As(1)	86.92(4)	Cl(1B)-Rh(1)-As(2)	93.15(4)
As(1)-Rh(1)-As(2)	176.134(9)	F(1)-B(1)-F(3)	108.4(2)
F(1)-B(1)-F(4)	109.8(3)	F(2)-B(1)-F(1)	109.4(2)
F(2)-B(1)-F(3)	109.5(3)	F(2)-B(1)-F(4)	110.3(2)
F(4)-B(1)-F(3)	109.4(2)	F(6)-B(2)-F(5)	108.7(2)
F(6)-B(2)-F(7)	111.2(3)	F(6)-B(2)-F(8)	109.5(2)
F(7)-B(2)-F(5)	109.7(2)	F(7)-B(2)-F(8)	109.3(2)
F(8)-B(2)-F(5)	108.5(2)		



Fully labeled solid-state structure of **17**.

Crystal data and structure refinement for 17.

CCDC	1408077	
Empirical formula	$C_{43}H_{39}As_2B_2ClF_{14}N_3ORh$	
Color	yellow-orange	
Formula weight	1189.59 g · mol^{-1}	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	ORTHORHOMBIC	
Space group	**Cmca, (no. 64)**	
Unit cell dimensions	a = 26.977(4) Å	α= 90°.
	b = 14.654(2) Å	β= 90°.
	c = 23.390(3) Å	γ = 90°.
Volume	9246(2) Å^3	
Z	8	
Density (calculated)	1.709 Mg · m^{-3}	
Absorption coefficient	1.943 mm^{-1}	
F(000)	4720 e	
Crystal size	0.16 x 0.13 x 0.06 mm^3	
θ range for data collection	2.780 to 33.287°.	
Index ranges	-41 ≤ h ≤ 41, -22≤ k ≤ 22, -36 ≤ l ≤ 36	
Reflections collected	149123	
Independent reflections	9049 [R_{int} = 0.1048]	
Reflections with I>2σ(I)	6243	
Completeness to θ = 25.242°	99.8 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.90 and 0.79	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9049 / 0 / 320	
Goodness-of-fit on F^2	1.087	
Final R indices [I>2σ(I)]	R_1 = 0.0368	wR^2 = 0.0777
R indices (all data)	R_1 = 0.0737	wR^2 = 0.0931
Largest diff. peak and hole	1.0 and -1.0 e · Å^{-3}	

Bond lengths [Å] and angles [°] for 17.

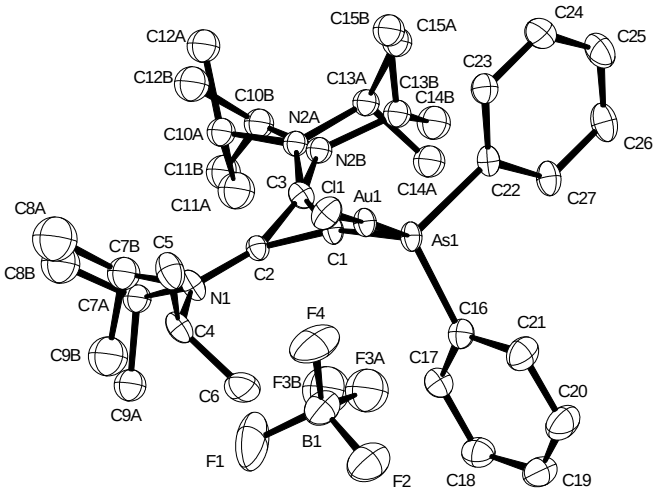
Rh(1)-As(1)	2.3820(4)	Rh(1)-As(1)*	2.3820(4)
Rh(1)-Cl(1)	2.3468(8)	Rh(1)-C(1)	1.825(3)
As(1)-C(2)	1.976(2)	As(1)-C(10)	1.933(2)
As(1)-C(16)	1.927(2)	F(1)-C(9)	1.331(3)
F(2)-C(9)	1.331(3)	F(3)-C(9)	1.332(3)
O(1)-C(1)	1.147(4)	N(1)-C(2)	1.365(3)
N(1)-C(6)	1.338(3)	N(1)-C(7)	1.501(3)
C(2)-C(3)	1.385(3)	C(3)-C(4)	1.392(3)
C(4)-C(5)	1.376(3)	C(5)-C(6)	1.377(3)
C(5)-C(9)	1.503(3)	C(7)-C(8)	1.502(3)
C(10)-C(11)	1.395(3)	C(10)-C(15)	1.395(3)
C(11)-C(12)	1.389(3)	C(12)-C(13)	1.384(3)
C(13)-C(14)	1.390(3)	C(14)-C(15)	1.392(3)
C(16)-C(17)	1.390(3)	C(16)-C(21)	1.393(3)
C(17)-C(18)	1.393(3)	C(18)-C(19)	1.386(3)
C(19)-C(20)	1.384(3)	C(20)-C(21)	1.386(3)
F(6)-B(2)	1.391(3)	F(7)-B(2)	1.379(5)
F(8)-B(2)	1.388(5)	B(2)-F(6)*	1.391(3)
F(4)-B(1)	1.368(3)	F(5)-B(1)	1.394(3)
B(1)-F(4)**	1.368(3)	B(1)-F(5)**	1.394(3)
N(99)-C(98)	1.140(5)	C(97)-C(98)	1.466(5)

As(1)*-Rh(1)-As(1)	172.166(14)	Cl(1)-Rh(1)-As(1)	91.197(8)
Cl(1)-Rh(1)-As(1)*	91.199(8)	C(1)-Rh(1)-As(1)*	89.467(11)
C(1)-Rh(1)-As(1)	89.469(11)	C(1)-Rh(1)-Cl(1)	169.98(10)
C(2)-As(1)-Rh(1)	116.23(6)	C(10)-As(1)-Rh(1)	118.46(7)
C(10)-As(1)-C(2)	100.15(9)	C(16)-As(1)-Rh(1)	113.65(7)
C(16)-As(1)-C(2)	100.40(9)	C(16)-As(1)-C(10)	105.59(9)
C(2)-N(1)-C(7)	123.09(18)	C(6)-N(1)-C(2)	121.06(19)
C(6)-N(1)-C(7)	115.84(18)	O(1)-C(1)-Rh(1)	175.8(3)
N(1)-C(2)-As(1)	121.24(15)	N(1)-C(2)-C(3)	118.71(19)
C(3)-C(2)-As(1)	120.02(16)	C(2)-C(3)-C(4)	120.9(2)
C(5)-C(4)-C(3)	118.3(2)	C(4)-C(5)-C(6)	119.9(2)
C(4)-C(5)-C(9)	122.0(2)	C(6)-C(5)-C(9)	118.1(2)
N(1)-C(6)-C(5)	121.2(2)	N(1)-C(7)-C(8)	111.89(19)

F(1)-C(9)-F(3)	107.0(2)	F(1)-C(9)-C(5)	111.7(2)
F(2)-C(9)-F(1)	107.0(2)	F(2)-C(9)-F(3)	107.1(2)
F(2)-C(9)-C(5)	112.05(19)	F(3)-C(9)-C(5)	111.7(2)
C(11)-C(10)-As(1)	121.01(16)	C(15)-C(10)-As(1)	118.97(16)
C(15)-C(10)-C(11)	120.0(2)	C(12)-C(11)-C(10)	119.8(2)
C(13)-C(12)-C(11)	120.2(2)	C(12)-C(13)-C(14)	120.2(2)
C(13)-C(14)-C(15)	120.1(2)	C(14)-C(15)-C(10)	119.6(2)
C(17)-C(16)-As(1)	116.64(16)	C(17)-C(16)-C(21)	120.4(2)
C(21)-C(16)-As(1)	122.93(17)	C(16)-C(17)-C(18)	119.5(2)
C(19)-C(18)-C(17)	120.1(2)	C(20)-C(19)-C(18)	120.2(2)
C(19)-C(20)-C(21)	120.4(2)	C(20)-C(21)-C(16)	119.5(2)
F(6)-B(2)-F(6)*	110.4(3)	F(7)-B(2)-F(6)*	109.0(2)
F(7)-B(2)-F(6)	109.0(2)	F(7)-B(2)-F(8)	110.6(3)
F(8)-B(2)-F(6)	108.9(2)	F(8)-B(2)-F(6)*	108.9(2)
F(4)-B(1)-F(4)**	109.9(3)	F(4)**-B(1)-F(5)	109.72(11)
F(4)**-B(1)-F(5)**	109.39(12)	F(4)-B(1)-F(5)	109.39(12)
F(4)-B(1)-F(5)**	109.73(11)	F(5)-B(1)-F(5)**	108.7(3)
N(99)-C(98)-C(97)	177.8(4)		

Symmetry transformations used to generate equivalent atoms:

* -x+1,y,z ** -x+1/2,y+0,-z+1/2



Fully labeled solid-state structure of **20**.

Crystal data and structure refinement for 20.

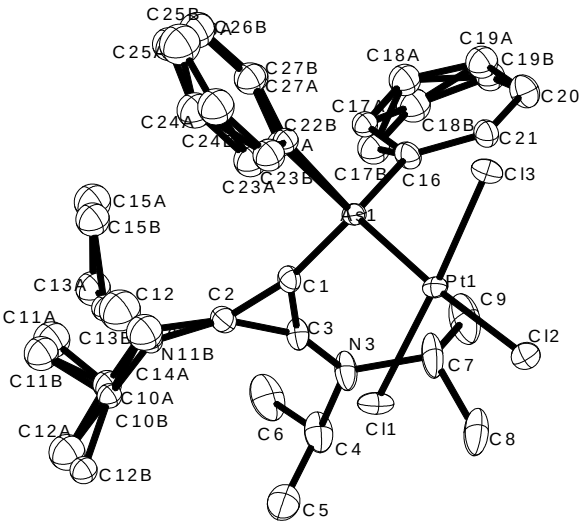
CCDC	1408071	
Empirical formula	$C_{27}H_{38}AsAuBClF_4N_2$	
Color	colorless	
Formula weight	784.74 g · mol^{-1}	
Temperature	100.15 K	
Wavelength	0.71073 Å	
Crystal system	MONOCLINIC	
Space group	**$P2_1/c$, (no. 14)**	
Unit cell dimensions	a = 10.7981(10) Å	α= 90°.
	b = 14.4676(4) Å	β= 102.129(8)°.
	c = 19.6810(10) Å	γ = 90°.
Volume	3006.0(4) Å^3	
Z	4	
Density (calculated)	1.734 Mg · m^{-3}	
Absorption coefficient	6.119 mm^{-1}	
F(000)	1536 e	
Crystal size	0.15 x 0.13 x 0.08 mm^3	
θ range for data collection	2.816 to 33.170°.	
Index ranges	-16 ≤ h ≤ 16, -22≤ k ≤ 22, -30 ≤ l ≤ 30	
Reflections collected	83084	
Independent reflections	11425 [R_{int} = 0.0428]	
Reflections with I>2σ(I)	10689	
Completeness to θ = 25.242°	99.2 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.79 and 0.47	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11425 / 0 / 338	
Goodness-of-fit on F^2	1.090	
Final R indices [I>2σ(I)]	R_1 = 0.0263	wR^2 = 0.0638
R indices (all data)	R_1 = 0.0287	wR^2 = 0.0654
Largest diff. peak and hole	1.0 and -1.9 e · Å^{-3}	

Bond lengths [Å] and angles [°] for 20.

Au(1)-As(1)	2.3361(2)	Au(1)-Cl(1)	2.2737(5)
As(1)-C(1)	1.910(2)	As(1)-C(16)	1.925(2)
As(1)-C(22)	1.921(2)	F(1)-B(1)	1.368(4)
F(2)-B(1)	1.377(4)	F(3A)-B(1)	1.441(5)
F(3B)-B(1)	1.329(11)	F(4)-B(1)	1.372(3)
N(1)-C(2)	1.306(3)	N(1)-C(4)	1.486(3)
N(1)-C(7A)	1.479(5)	N(1)-C(7B)	1.530(7)
N(2A)-C(3)	1.358(4)	N(2A)-C(10A)	1.489(7)
N(2A)-C(13A)	1.490(6)	N(2B)-C(3)	1.273(4)
N(2B)-C(10B)	1.492(7)	N(2B)-C(13B)	1.490(6)
C(1)-C(2)	1.378(3)	C(1)-C(3)	1.384(3)
C(2)-C(3)	1.415(3)	C(4)-C(5)	1.519(4)
C(4)-C(6)	1.523(4)	C(7A)-C(8A)	1.491(10)
C(7A)-C(9A)	1.542(9)	C(7B)-C(8B)	1.486(14)
C(7B)-C(9B)	1.573(13)	C(10A)-C(11A)	1.562(9)
C(10A)-C(12A)	1.528(7)	C(10B)-C(11B)	1.524(9)
C(10B)-C(12B)	1.516(8)	C(13A)-C(14A)	1.521(7)
C(13A)-C(15A)	1.529(9)	C(13B)-C(14B)	1.515(8)
C(13B)-C(15B)	1.531(9)	C(16)-C(17)	1.390(3)
C(16)-C(21)	1.395(3)	C(17)-C(18)	1.394(4)
C(18)-C(19)	1.386(4)	C(19)-C(20)	1.385(4)
C(20)-C(21)	1.394(4)	C(22)-C(23)	1.390(3)
C(22)-C(27)	1.396(3)	C(23)-C(24)	1.389(4)
C(24)-C(25)	1.393(4)	C(25)-C(26)	1.377(4)
C(26)-C(27)	1.389(4)		

Cl(1)-Au(1)-As(1)	176.293(16)	C(1)-As(1)-Au(1)	113.94(6)
C(1)-As(1)-C(16)	103.91(9)	C(1)-As(1)-C(22)	106.74(9)
C(16)-As(1)-Au(1)	114.95(7)	C(22)-As(1)-Au(1)	112.30(7)
C(22)-As(1)-C(16)	104.05(10)	C(2)-N(1)-C(4)	121.61(19)
C(2)-N(1)-C(7A)	120.3(2)	C(2)-N(1)-C(7B)	119.6(3)
C(4)-N(1)-C(7B)	117.8(3)	C(7A)-N(1)-C(4)	117.2(2)
C(3)-N(2A)-C(10A)	121.4(4)	C(3)-N(2A)-C(13A)	119.8(4)
C(10A)-N(2A)-C(13A)	118.6(4)	C(3)-N(2B)-C(10B)	121.0(4)
C(3)-N(2B)-C(13B)	119.6(4)	C(13B)-N(2B)-C(10B)	118.7(4)
C(2)-C(1)-As(1)	146.31(16)	C(2)-C(1)-C(3)	61.61(15)

C(3)-C(1)-As(1)	151.05(17)	N(1)-C(2)-C(1)	150.5(2)
N(1)-C(2)-C(3)	150.1(2)	C(1)-C(2)-C(3)	59.40(15)
N(2A)-C(3)-C(1)	157.2(3)	N(2A)-C(3)-C(2)	142.7(3)
N(2B)-C(3)-C(1)	141.6(3)	N(2B)-C(3)-C(2)	159.2(3)
C(1)-C(3)-C(2)	58.99(14)	N(1)-C(4)-C(5)	110.8(2)
N(1)-C(4)-C(6)	111.8(2)	C(5)-C(4)-C(6)	112.0(2)
N(1)-C(7A)-C(8A)	109.6(5)	N(1)-C(7A)-C(9A)	112.1(4)
C(8A)-C(7A)-C(9A)	112.0(5)	N(1)-C(7B)-C(9B)	104.1(7)
C(8B)-C(7B)-N(1)	113.7(7)	C(8B)-C(7B)-C(9B)	113.5(7)
N(2A)-C(10A)-C(11A)	97.8(4)	N(2A)-C(10A)-C(12A)	110.7(4)
C(12A)-C(10A)-C(11A)	126.0(5)	N(2B)-C(10B)-C(11B)	125.9(5)
N(2B)-C(10B)-C(12B)	111.4(4)	C(12B)-C(10B)-C(11B)	106.3(5)
N(2A)-C(13A)-C(14A)	109.7(4)	N(2A)-C(13A)-C(15A)	113.8(4)
C(14A)-C(13A)-C(15A)	109.9(5)	N(2B)-C(13B)-C(14B)	110.9(4)
N(2B)-C(13B)-C(15B)	107.7(5)	C(14B)-C(13B)-C(15B)	115.4(5)
C(17)-C(16)-As(1)	123.20(17)	C(17)-C(16)-C(21)	120.8(2)
C(21)-C(16)-As(1)	116.03(18)	C(16)-C(17)-C(18)	118.9(2)
C(19)-C(18)-C(17)	120.4(3)	C(20)-C(19)-C(18)	120.7(3)
C(19)-C(20)-C(21)	119.4(3)	C(20)-C(21)-C(16)	119.8(3)
C(23)-C(22)-As(1)	118.48(16)	C(23)-C(22)-C(27)	120.7(2)
C(27)-C(22)-As(1)	120.78(18)	C(24)-C(23)-C(22)	119.4(2)
C(23)-C(24)-C(25)	119.8(3)	C(26)-C(25)-C(24)	120.6(3)
C(25)-C(26)-C(27)	120.2(2)	C(26)-C(27)-C(22)	119.2(2)
F(1)-B(1)-F(2)	108.4(3)	F(1)-B(1)-F(3A)	113.1(3)
F(1)-B(1)-F(4)	112.3(3)	F(2)-B(1)-F(3A)	101.2(3)
F(3B)-B(1)-F(1)	86.7(5)	F(3B)-B(1)-F(2)	123.9(5)
F(3B)-B(1)-F(4)	112.7(5)	F(4)-B(1)-F(2)	110.2(2)
F(4)-B(1)-F(3A)	111.1(3)		



Fully labeled solid-state structure of **25**.

Crystal data and structure refinement for 25.

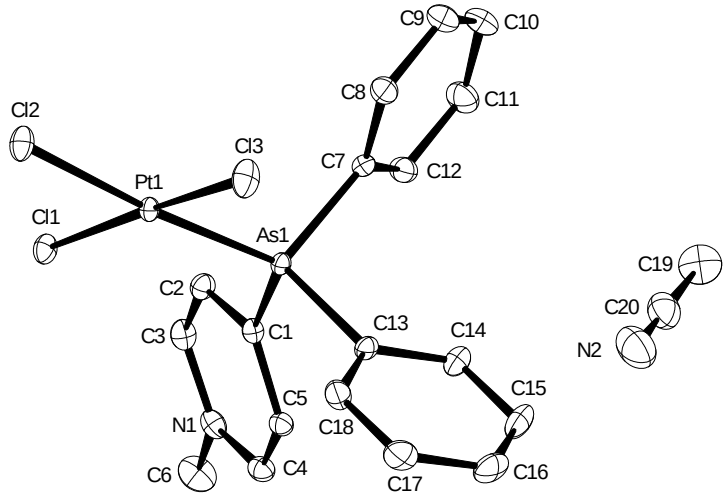
CCDC	1408072	
Empirical formula	$C_{27}H_{38}AsCl_3N_2Pt$	
Color	orange	
Formula weight	766.95 g·mol^{-1}	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	MONOCLINIC	
Space group	c c, (no. 9)	
Unit cell dimensions	a = 13.703(3) Å	α= 90°.
	b = 15.618(3) Å	β= 90.12(3)°.
	c = 16.178(3) Å	γ = 90°.
Volume	3462.3(12) Å^3	
Z	4	
Density (calculated)	1.471 Mg·m^{-3}	
Absorption coefficient	5.248 mm^{-1}	
F(000)	1504 e	
Crystal size	0.20 x 0.14 x 0.10 mm^3	
θ range for data collection	2.608 to 29.980°.	
Index ranges	-19 ≤ h ≤ 19, -21≤ k ≤ 21, -22≤ l ≤ 22	
Reflections collected	63300	
Independent reflections	9967 [R_{int} = 0.0235]	
Reflections with I>2σ(I)	9911	
Completeness to θ = 25.242°	99.0 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.37805 and 0.21886	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9967 / 10 / 279	
Goodness-of-fit on F^2	1.070	
Final R indices [I>2σ(I)]	R_1 = 0.0201	wR^2 = 0.0576
R indices (all data)	R_1 = 0.0203	wR^2 = 0.0577
Absolute structure parameter	-0.001(3)	
Extinction coefficient	0	
Largest diff. peak and hole	0.921 and -0.928 e·Å^{-3}	

Selected bond lengths [Å] and angles [°] for 25.

As(1)-C(1)	1.933(4)	As(1)-C(16)	1.929(4)
As(1)-C(22B)	1.942(6)	As(1)-Pt(1)	2.3206(8)
As(1)-C(22A)	1.887(5)	C(1)-C(2)	1.374(6)
C(1)-C(3)	1.379(6)	C(2)-C(3)	1.411(6)
C(2)-N(11B)	1.315(8)	C(2)-N(11A)	1.345(9)
C(3)-N(3)	1.302(6)	C(4)-C(5)	1.533(9)
C(4)-C(6)	1.514(9)	C(4)-N(3)	1.490(6)
C(7)-C(8)	1.544(9)	C(7)-C(9)	1.508(9)
C(7)-N(3)	1.490(6)	C(10B)-C(11B)	1.521(10)
C(10B)-C(12B)	1.491(10)	C(10B)-N(11B)	1.502(11)
C(13B)-C(15B)	1.527(10)	C(13B)-N(11B)	1.485(11)
C(13B)-C(14A)	1.516(10)	C(16)-C(17B)	1.403(12)
C(16)-C(21)	1.384(6)	C(16)-C(17A)	1.421(10)
C(17B)-C(18B)	1.395(16)	C(18B)-C(19B)	1.407(17)
C(19B)-C(20)	1.361(13)	C(20)-C(21)	1.383(6)
C(20)-C(19A)	1.415(15)	Cl(1)-Pt(1)	2.3064(11)
Cl(2)-Pt(1)	2.3221(19)	Cl(3)-Pt(1)	2.3115(11)
C(19A)-C(18A)	1.341(18)	C(18A)-C(17A)	1.391(14)
N(11A)-C(13A)	1.505(14)	N(11A)-C(10A)	1.489(13)
C(13A)-C(15A)	1.499(11)	C(13A)-C(12)	1.497(12)
C(10A)-C(12A)	1.499(11)	C(10A)-C(11A)	1.507(11)
C(1)-As(1)-C(22B)	108.2(3)	C(1)-As(1)-Pt(1)	112.63(13)
C(16)-As(1)-C(1)	98.27(18)	C(16)-As(1)-C(22B)	106.9(3)
C(16)-As(1)-Pt(1)	115.53(13)	C(22B)-As(1)-Pt(1)	114.0(2)
C(22A)-As(1)-C(1)	102.4(3)	C(22A)-As(1)-C(16)	105.4(3)
C(22A)-As(1)-Pt(1)	119.8(3)	C(2)-C(1)-As(1)	158.0(3)
C(2)-C(1)-C(3)	61.6(3)	C(3)-C(1)-As(1)	139.3(3)
C(1)-C(2)-C(3)	59.4(3)	N(11B)-C(2)-C(1)	146.0(5)
N(11B)-C(2)-C(3)	151.0(5)	N(11A)-C(2)-C(1)	153.1(5)
N(11A)-C(2)-C(3)	145.7(6)	C(1)-C(3)-C(2)	59.0(3)
N(3)-C(3)-C(1)	146.9(4)	N(3)-C(3)-C(2)	154.0(4)
C(6)-C(4)-C(5)	115.8(4)	N(3)-C(4)-C(5)	110.3(4)
N(3)-C(4)-C(6)	111.7(5)	C(9)-C(7)-C(8)	112.7(5)
N(3)-C(7)-C(8)	110.2(5)	N(3)-C(7)-C(9)	110.9(5)
C(12B)-C(10B)-C(11B)	112.1(7)	C(12B)-C(10B)-N(11B)	111.8(7)

N(11B)-C(10B)-C(11B)	110.5(7)	N(11B)-C(13B)-C(15B)	111.9(8)
N(11B)-C(13B)-C(14A)	107.8(8)	C(14A)-C(13B)-C(15B)	114.6(8)
C(17B)-C(16)-As(1)	119.9(5)	C(21)-C(16)-As(1)	120.4(3)
C(21)-C(16)-C(17B)	118.5(6)	C(21)-C(16)-C(17A)	118.6(5)
C(17A)-C(16)-As(1)	120.3(4)	C(18B)-C(17B)-C(16)	119.2(10)
C(17B)-C(18B)-C(19B)	120.8(11)	C(20)-C(19B)-C(18B)	118.3(11)
C(19B)-C(20)-C(21)	121.7(7)	C(21)-C(20)-C(19A)	119.9(7)
C(20)-C(21)-C(16)	120.4(4)	C(23B)-C(22B)-As(1)	118.4(4)
C(27B)-C(22B)-As(1)	121.5(4)	C(3)-N(3)-C(4)	122.4(4)
C(3)-N(3)-C(7)	118.8(4)	C(7)-N(3)-C(4)	118.7(4)
C(2)-N(11B)-C(10B)	117.9(6)	C(2)-N(11B)-C(13B)	123.6(6)
C(13B)-N(11B)-C(10B)	118.1(7)	As(1)-Pt(1)-Cl(2)	174.85(3)
Cl(1)-Pt(1)-As(1)	91.72(4)	Cl(1)-Pt(1)-Cl(2)	91.03(5)
Cl(1)-Pt(1)-Cl(3)	175.02(4)	Cl(3)-Pt(1)-As(1)	88.63(4)
Cl(3)-Pt(1)-Cl(2)	89.01(6)	C(23A)-C(22A)-As(1)	118.1(4)
C(27A)-C(22A)-As(1)	121.9(4)	C(18A)-C(19A)-C(20)	119.4(12)
C(19A)-C(18A)-C(17A)	122.0(11)	C(18A)-C(17A)-C(16)	119.1(8)
C(2)-N(11A)-C(13A)	117.4(8)	C(2)-N(11A)-C(10A)	123.9(7)
C(10A)-N(11A)-C(13A)	118.6(8)	C(15A)-C(13A)-N(11A)	109.9(10)
C(12)-C(13A)-N(11A)	108.7(10)	C(12)-C(13A)-C(15A)	114.6(11)
N(11A)-C(10A)-C(12A)	112.1(9)	N(11A)-C(10A)-C(11A)	110.3(8)
C(12A)-C(10A)-C(11A)	112.1(9)		

Symmetry transformations used to generate equivalent atoms:



Fully labeled solid-state structure of **26**.

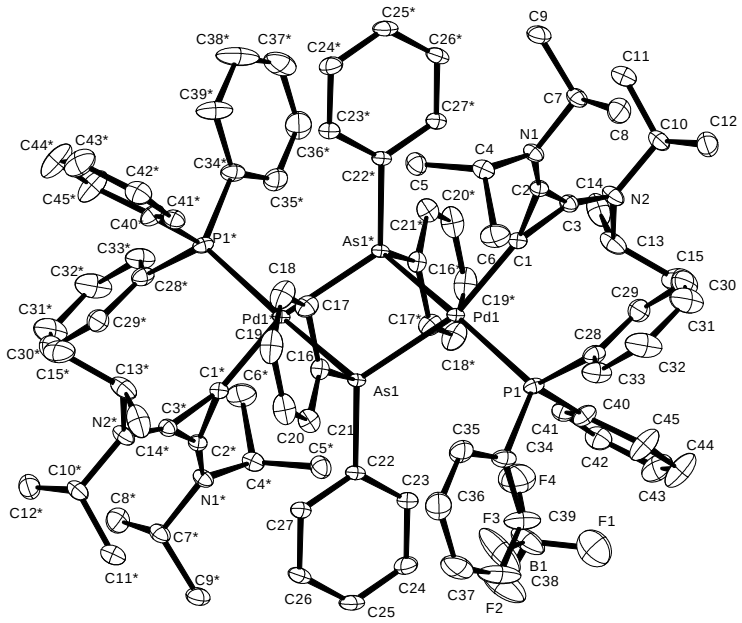
Crystal data and structure refinement for 26.

CCDC	1472101	
Empirical formula	$C_{20}H_{20}AsCl_3N_2Pt$	
Color	yellow	
Formula weight	664.74 $g \cdot mol^{-1}$	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	MONOCLINIC	
Space group	p 21/n, (no. 14)	
Unit cell dimensions	a = 15.897(2) Å	α= 90°.
	b = 8.9367(13) Å	β= 108.911(2)°.
	c = 16.166(2) Å	γ = 90°.
Volume	2172.7(6) $Å^3$	
Z	4	
Density (calculated)	2.032 $Mg \cdot m^{-3}$	
Absorption coefficient	8.346 mm^{-1}	
F(000)	1264 e	
Crystal size	0.201 x 0.125 x 0.060 mm^3	
θ range for data collection	3.124 to 33.998°.	
Index ranges	$-24 \le h \le 24$, $-14 \le k \le 14$, $-25 \le l \le 25$	
Reflections collected	128075	
Independent reflections	8831 [R_{int} = 0.0386]	
Reflections with I>2σ(I)	8053	
Completeness to θ = 25.242°	99.8 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.71916 and 0.30039	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8831 / 0 / 246	
Goodness-of-fit on F^2	1.030	
Final R indices [I>2σ(I)]	R_1 = 0.0154	wR^2 = 0.0339
R indices (all data)	R_1 = 0.0192	wR^2 = 0.0350
Extinction coefficient	n/a	
Largest diff. peak and hole	1.756 and -0.846 $e \cdot Å^{-3}$	

Bond lengths [Å] and angles [°] for 26.

Pt(1)-As(1)	2.3348(3)	Pt(1)-Cl(1)	2.2917(4)
Pt(1)-Cl(3)	2.3012(4)	Pt(1)-Cl(2)	2.3390(4)
As(1)-C(7)	1.9330(15)	As(1)-C(1)	1.9478(14)
As(1)-C(13)	1.9291(14)	C(7)-C(12)	1.388(2)
C(7)-C(8)	1.396(2)	N(1)-C(4)	1.345(2)
N(1)-C(3)	1.349(2)	N(1)-C(6)	1.478(2)
C(12)-C(11)	1.394(2)	C(11)-C(10)	1.388(2)
C(1)-C(5)	1.392(2)	C(1)-C(2)	1.395(2)
C(5)-C(4)	1.383(2)	C(8)-C(9)	1.392(2)
C(10)-C(9)	1.383(3)	C(13)-C(18)	1.387(2)
C(13)-C(14)	1.395(2)	N(2)-C(20)	1.138(3)
C(3)-C(2)	1.376(2)	C(18)-C(17)	1.392(2)
C(19)-C(20)	1.449(3)	C(14)-C(15)	1.390(2)
C(17)-C(16)	1.385(3)	C(16)-C(15)	1.386(3)

As(1)-Pt(1)-Cl(2)	175.785(11)	Cl(1)-Pt(1)-As(1)	93.787(13)
Cl(1)-Pt(1)-Cl(3)	174.629(15)	Cl(1)-Pt(1)-Cl(2)	87.916(16)
Cl(3)-Pt(1)-As(1)	89.064(14)	Cl(3)-Pt(1)-Cl(2)	89.551(17)
C(7)-As(1)-Pt(1)	114.56(4)	C(7)-As(1)-C(1)	101.16(6)
C(1)-As(1)-Pt(1)	115.23(4)	C(13)-As(1)-Pt(1)	118.17(5)
C(13)-As(1)-C(7)	102.75(6)	C(13)-As(1)-C(1)	102.71(6)
C(12)-C(7)-As(1)	121.30(11)	C(12)-C(7)-C(8)	120.61(14)
C(8)-C(7)-As(1)	118.09(12)	C(4)-N(1)-C(3)	121.20(13)
C(4)-N(1)-C(6)	118.66(14)	C(3)-N(1)-C(6)	120.11(14)
C(7)-C(12)-C(11)	119.71(15)	C(10)-C(11)-C(12)	119.72(16)
C(5)-C(1)-As(1)	120.97(11)	C(5)-C(1)-C(2)	118.72(13)
C(2)-C(1)-As(1)	120.31(11)	C(4)-C(5)-C(1)	119.28(14)
N(1)-C(4)-C(5)	120.67(14)	C(9)-C(8)-C(7)	119.18(16)
C(9)-C(10)-C(11)	120.49(15)	C(18)-C(13)-As(1)	120.09(11)
C(18)-C(13)-C(14)	120.65(14)	C(14)-C(13)-As(1)	119.26(11)
N(1)-C(3)-C(2)	120.26(14)	C(13)-C(18)-C(17)	119.63(15)
C(3)-C(2)-C(1)	119.86(14)	N(2)-C(20)-C(19)	179.6(2)
C(10)-C(9)-C(8)	120.28(15)	C(15)-C(14)-C(13)	119.32(16)
C(16)-C(17)-C(18)	119.78(16)	C(17)-C(16)-C(15)	120.65(15)
C(16)-C(15)-C(14)	119.96(16)		



Fully labeled solid-state structure of **27**.

Crystal data and structure refinement for 27.

CCDC	1408076	
Empirical formula	$C_{90}H_{106}As_2B_2F_8N_4P_2Pd_2$	
Color	yellow	
Formula weight	1841.98 g · mol^{-1}	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	TRICLINIC	
Space group	**P$\bar{1}$, (no. 2)**	
Unit cell dimensions	a = 13.952(3) Å	α= 91.716(3)°.
	b = 14.156(3) Å	β= 117.853(3)°.
	c = 14.899(3) Å	γ = 94.200(3)°.
Volume	2587.9(8) Å^3	
Z	1	
Density (calculated)	1.182 Mg · m^{-3}	
Absorption coefficient	1.066 mm^{-1}	
F(000)	944 e	
Crystal size	0.17 x 0.10 x 0.09 mm^3	
θ range for data collection	2.306 to 33.287°.	
Index ranges	$-21 \le h \le 21$, $-21 \le k \le 21$, $-22 \le l \le 22$	
Reflections collected	86714	
Independent reflections	19810 [R_{int} = 0.0327]	
Reflections with I>2σ(I)	16973	
Completeness to θ = 25.242°	99.7 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.92 and 0.83	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	19810 / 0 / 504	
Goodness-of-fit on F^2	1.097	
Final R indices [I>2σ(I)]	R_1 = 0.0290	wR^2 = 0.0858
R indices (all data)	R_1 = 0.0349	wR^2 = 0.0884
Largest diff. peak and hole	0.8 and -0.8 e · Å^{-3}	

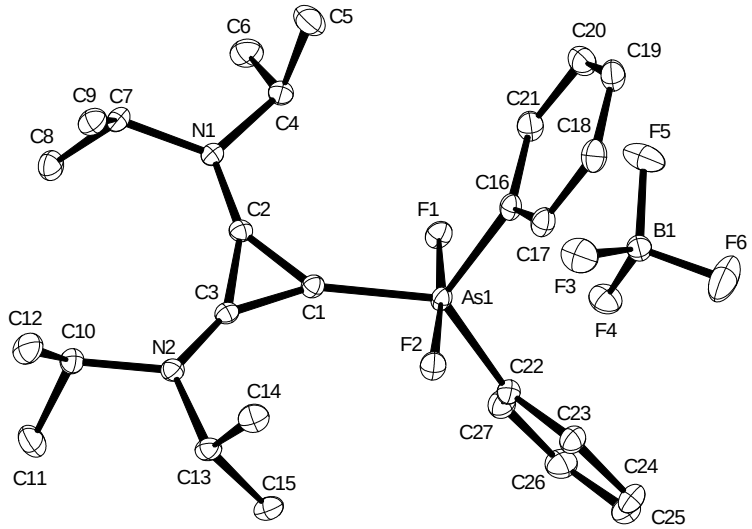
Bond lengths [Å] and angles [°] for 27.

Pd(1)-As(1)*	2.4663(3)	Pd(1)-As(1)	2.4664(3)
Pd(1)-P(1)	2.3607(5)	Pd(1)-C(1)	2.0082(14)
As(1)-Pd(1)*	2.4664(3)	As(1)-C(16)	1.9488(13)
As(1)-C(22)	1.9391(13)	P(1)-C(28)	1.8318(16)
P(1)-C(34)	1.8176(15)	P(1)-C(40)	1.8219(15)
N(1)-C(2)	1.3220(17)	N(1)-C(4)	1.4821(17)
N(1)-C(7)	1.4783(18)	N(2)-C(3)	1.3252(17)
N(2)-C(10)	1.4856(19)	N(2)-C(13)	1.4851(19)
C(1)-C(2)	1.3926(19)	C(1)-C(3)	1.3856(18)
C(2)-C(3)	1.3941(18)	C(4)-C(5)	1.520(2)
C(4)-C(6)	1.520(2)	C(7)-C(8)	1.519(2)
C(7)-C(9)	1.529(2)	C(10)-C(11)	1.519(2)
C(10)-C(12)	1.521(2)	C(13)-C(14)	1.520(3)
C(13)-C(15)	1.529(3)	C(16)-C(17)	1.401(2)
C(16)-C(21)	1.3978(19)	C(17)-C(18)	1.391(2)
C(18)-C(19)	1.392(3)	C(19)-C(20)	1.382(3)
C(20)-C(21)	1.402(2)	C(22)-C(23)	1.3919(19)
C(22)-C(27)	1.3975(19)	C(23)-C(24)	1.395(2)
C(24)-C(25)	1.394(2)	C(25)-C(26)	1.386(2)
C(26)-C(27)	1.399(2)	C(28)-C(29)	1.394(2)
C(28)-C(33)	1.401(2)	C(29)-C(30)	1.392(2)
C(30)-C(31)	1.386(3)	C(31)-C(32)	1.378(3)
C(32)-C(33)	1.398(3)	C(34)-C(35)	1.389(2)
C(34)-C(39)	1.398(2)	C(35)-C(36)	1.395(2)
C(36)-C(37)	1.383(3)	C(37)-C(38)	1.397(3)
C(38)-C(39)	1.383(3)	C(40)-C(41)	1.394(2)
C(40)-C(45)	1.402(2)	C(41)-C(42)	1.389(2)
C(42)-C(43)	1.389(3)	C(43)-C(44)	1.394(3)
C(44)-C(45)	1.391(3)	F(1)-B(1)	1.386(3)
F(2)-B(1)	1.379(2)	F(3)-B(1)	1.393(2)
F(4)-B(1)	1.387(3)		

As(1)*-Pd(1)-As(1)	75.311(13)	P(1)-Pd(1)-As(1)	103.904(16)
P(1)-Pd(1)-As(1)*	167.741(10)	C(1)-Pd(1)-As(1)	163.21(4)
C(1)-Pd(1)-As(1)*	92.57(4)	C(1)-Pd(1)-P(1)	90.40(4)
Pd(1)-As(1)-Pd(1)*	104.688(13)	C(16)-As(1)-Pd(1)	103.14(4)
C(16)-As(1)-Pd(1)*	101.58(4)	C(22)-As(1)-Pd(1)*	115.00(4)
C(22)-As(1)-Pd(1)	124.06(4)	C(22)-As(1)-C(16)	105.51(6)
C(28)-P(1)-Pd(1)	118.97(5)	C(34)-P(1)-Pd(1)	116.83(5)
C(34)-P(1)-C(28)	103.55(7)	C(34)-P(1)-C(40)	104.78(7)
C(40)-P(1)-Pd(1)	109.17(5)	C(40)-P(1)-C(28)	101.70(7)
C(2)-N(1)-C(4)	119.59(12)	C(2)-N(1)-C(7)	121.97(11)
C(7)-N(1)-C(4)	118.42(11)	C(3)-N(2)-C(10)	123.32(12)
C(3)-N(2)-C(13)	117.47(12)	C(13)-N(2)-C(10)	119.09(11)
C(2)-C(1)-Pd(1)	147.44(10)	C(3)-C(1)-Pd(1)	152.31(10)
C(3)-C(1)-C(2)	60.24(9)	N(1)-C(2)-C(1)	148.54(13)
N(1)-C(2)-C(3)	151.81(13)	C(1)-C(2)-C(3)	59.63(9)

N(2)-C(3)-C(1)	145.80(13)	N(2)-C(3)-C(2)	154.01(14)
C(1)-C(3)-C(2)	60.13(9)	N(1)-C(4)-C(5)	111.08(12)
N(1)-C(4)-C(6)	111.45(12)	C(5)-C(4)-C(6)	111.87(14)
N(1)-C(7)-C(8)	111.31(12)	N(1)-C(7)-C(9)	111.05(12)
C(8)-C(7)-C(9)	112.33(12)	N(2)-C(10)-C(11)	111.46(12)
N(2)-C(10)-C(12)	111.39(12)	C(11)-C(10)-C(12)	114.11(13)
N(2)-C(13)-C(14)	110.99(14)	N(2)-C(13)-C(15)	110.77(15)
C(14)-C(13)-C(15)	111.51(13)	C(17)-C(16)-As(1)	117.87(10)
C(21)-C(16)-As(1)	123.06(11)	C(21)-C(16)-C(17)	119.01(13)
C(18)-C(17)-C(16)	120.78(15)	C(17)-C(18)-C(19)	119.73(16)
C(20)-C(19)-C(18)	120.22(14)	C(19)-C(20)-C(21)	120.31(15)
C(16)-C(21)-C(20)	119.95(15)	C(23)-C(22)-As(1)	118.56(10)
C(23)-C(22)-C(27)	119.65(12)	C(27)-C(22)-As(1)	121.46(10)
C(22)-C(23)-C(24)	120.60(13)	C(25)-C(24)-C(23)	119.52(13)
C(26)-C(25)-C(24)	120.25(13)	C(25)-C(26)-C(27)	120.24(13)
C(22)-C(27)-C(26)	119.73(13)	C(29)-C(28)-P(1)	117.60(11)
C(29)-C(28)-C(33)	118.99(15)	C(33)-C(28)-P(1)	123.40(12)
C(30)-C(29)-C(28)	120.54(16)	C(31)-C(30)-C(29)	120.12(18)
C(32)-C(31)-C(30)	119.96(17)	C(31)-C(32)-C(33)	120.55(17)
C(32)-C(33)-C(28)	119.82(17)	C(35)-C(34)-P(1)	118.37(11)
C(35)-C(34)-C(39)	119.54(14)	C(39)-C(34)-P(1)	122.10(13)
C(34)-C(35)-C(36)	120.04(17)	C(37)-C(36)-C(35)	120.23(19)
C(36)-C(37)-C(38)	119.94(16)	C(39)-C(38)-C(37)	119.91(18)
C(38)-C(39)-C(34)	120.34(18)	C(41)-C(40)-P(1)	119.83(11)
C(41)-C(40)-C(45)	119.41(14)	C(45)-C(40)-P(1)	120.72(12)
C(42)-C(41)-C(40)	120.81(15)	C(43)-C(42)-C(41)	119.66(16)
C(42)-C(43)-C(44)	119.99(16)	C(45)-C(44)-C(43)	120.49(18)
C(44)-C(45)-C(40)	119.57(18)	F(1)-B(1)-F(3)	108.4(2)
F(1)-B(1)-F(4)	107.03(17)	F(2)-B(1)-F(1)	109.73(18)
F(2)-B(1)-F(3)	110.36(16)	F(2)-B(1)-F(4)	110.1(2)
F(4)-B(1)-F(3)	111.19(19)		

Symmetry transformations used to generate equivalent atoms: * -x+1,-y+1,-z+1



Fully labeled solid-state structure of **28**.

Crystal data and structure refinement for 28.

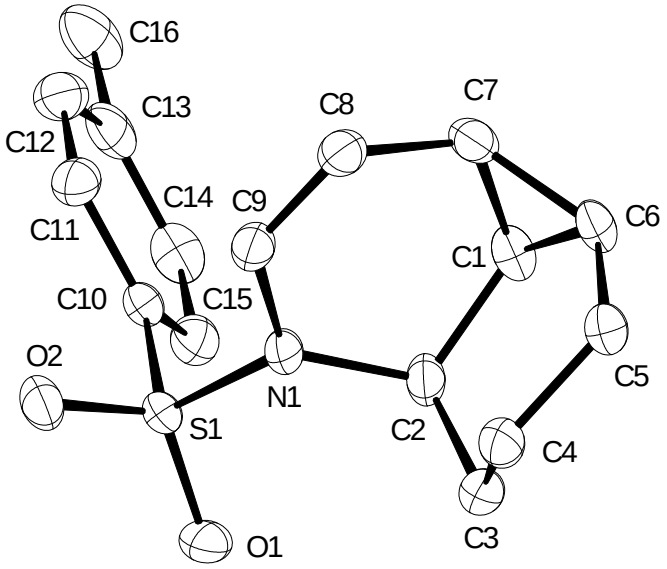
CCDC	1408079	
Empirical formula	$C_{27}H_{38}AsBF_6N_2$	
Color	colorless	
Formula weight	590.32 g · mol^{-1}	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	**Pbca, (no. 61)**	
Unit cell dimensions	a = 15.962(2) Å	α= 90°.
	b = 11.9347(18) Å	β= 90°.
	c = 29.201(5) Å	γ = 90°.
Volume	5562.7(15) Å^3	
Z	8	
Density (calculated)	1.410 Mg · m^{-3}	
Absorption coefficient	1.281 mm^{-1}	
F(000)	2448 e	
Crystal size	0.22 x 0.09 x 0.04 mm^3	
θ range for data collection	2.909 to 33.298°.	
Index ranges	-24 ≤ h ≤ 24, -18≤ k ≤ 18, -45 ≤ l ≤ 45	
Reflections collected	180257	
Independent reflections	10737 [R_{int} = 0.1025]	
Reflections with I>2σ(I)	7672	
Completeness to θ = 25.242°	99.9 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.95 and 0.76	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10737 / 0 / 342	
Goodness-of-fit on F^2	1.027	
Final R indices [I>2σ(I)]	R_1 = 0.0352	wR^2 = 0.0696
R indices (all data)	R_1 = 0.0660	wR^2 = 0.0796
Largest diff. peak and hole	0.4 and -0.5 e · Å^{-3}	

Bond lengths [Å] and angles [°] for 28.

As(1)-F(1)	1.8114(9)	As(1)-F(2)	1.8103(9)
As(1)-C(1)	1.9053(14)	As(1)-C(16)	1.9246(15)
As(1)-C(22)	1.9165(14)	N(1)-C(2)	1.3077(17)
N(1)-C(4)	1.4948(18)	N(1)-C(7)	1.4904(18)
N(2)-C(3)	1.3030(17)	N(2)-C(10)	1.4883(19)
N(2)-C(13)	1.4943(18)	C(1)-C(2)	1.3777(19)
C(1)-C(3)	1.3824(19)	C(2)-C(3)	1.4261(19)
C(4)-C(5)	1.523(2)	C(4)-C(6)	1.522(2)
C(7)-C(8)	1.525(2)	C(7)-C(9)	1.522(2)
C(10)-C(11)	1.523(2)	C(10)-C(12)	1.523(2)
C(13)-C(14)	1.528(2)	C(13)-C(15)	1.521(2)
C(16)-C(17)	1.394(2)	C(16)-C(21)	1.396(2)
C(17)-C(18)	1.387(2)	C(18)-C(19)	1.384(2)
C(19)-C(20)	1.382(2)	C(20)-C(21)	1.387(2)
C(22)-C(23)	1.393(2)	C(22)-C(27)	1.387(2)
C(23)-C(24)	1.388(2)	C(24)-C(25)	1.384(3)
C(25)-C(26)	1.384(2)	C(26)-C(27)	1.391(2)
F(3)-B(1)	1.3961(19)	F(4)-B(1)	1.3998(19)
F(5)-B(1)	1.3963(19)	F(6)-B(1)	1.381(2)

F(1)-As(1)-C(1)	86.51(5)	F(1)-As(1)-C(16)	92.61(5)
F(1)-As(1)-C(22)	89.58(5)	F(2)-As(1)-F(1)	174.43(4)
F(2)-As(1)-C(1)	88.45(5)	F(2)-As(1)-C(16)	91.79(5)
F(2)-As(1)-C(22)	91.46(5)	C(1)-As(1)-C(16)	116.91(6)
C(1)-As(1)-C(22)	125.98(6)	C(22)-As(1)-C(16)	117.08(6)
C(2)-N(1)-C(4)	118.17(12)	C(2)-N(1)-C(7)	122.79(12)
C(7)-N(1)-C(4)	118.32(11)	C(3)-N(2)-C(10)	121.04(12)
C(3)-N(2)-C(13)	121.44(12)	C(10)-N(2)-C(13)	117.45(11)
C(2)-C(1)-As(1)	144.92(11)	C(2)-C(1)-C(3)	62.22(10)
C(3)-C(1)-As(1)	152.48(11)	N(1)-C(2)-C(1)	148.40(13)
N(1)-C(2)-C(3)	152.36(13)	C(1)-C(2)-C(3)	59.05(9)
N(2)-C(3)-C(1)	151.11(14)	N(2)-C(3)-C(2)	150.16(13)
C(1)-C(3)-C(2)	58.73(9)	N(1)-C(4)-C(5)	109.80(12)
N(1)-C(4)-C(6)	112.03(12)	C(6)-C(4)-C(5)	112.40(13)
N(1)-C(7)-C(8)	111.23(12)	N(1)-C(7)-C(9)	111.15(12)

C(9)-C(7)-C(8)	114.99(12)	N(2)-C(10)-C(11)	110.75(12)
N(2)-C(10)-C(12)	111.18(13)	C(11)-C(10)-C(12)	112.11(13)
N(2)-C(13)-C(14)	110.49(12)	N(2)-C(13)-C(15)	111.31(12)
C(15)-C(13)-C(14)	114.00(12)	C(17)-C(16)-As(1)	120.27(11)
C(17)-C(16)-C(21)	120.29(14)	C(21)-C(16)-As(1)	119.42(12)
C(18)-C(17)-C(16)	119.53(14)	C(19)-C(18)-C(17)	120.09(15)
C(20)-C(19)-C(18)	120.45(15)	C(19)-C(20)-C(21)	120.23(15)
C(20)-C(21)-C(16)	119.39(15)	C(23)-C(22)-As(1)	117.71(12)
C(27)-C(22)-As(1)	120.95(11)	C(27)-C(22)-C(23)	120.87(14)
C(24)-C(23)-C(22)	119.50(15)	C(25)-C(24)-C(23)	119.94(15)
C(24)-C(25)-C(26)	120.25(15)	C(25)-C(26)-C(27)	120.53(16)
C(22)-C(27)-C(26)	118.90(15)	F(3)-B(1)-F(4)	109.13(12)
F(5)-B(1)-F(3)	108.83(13)	F(5)-B(1)-F(4)	108.84(13)
F(6)-B(1)-F(3)	109.60(14)	F(6)-B(1)-F(4)	110.29(13)
F(6)-B(1)-F(5)	110.12(13)		



Fully labeled solid-state structure of **31**.

Crystal data and structure refinement for 31.

CCDC	1472098	
Empirical formula	$C_{16}H_{19}NO_2S$	
Color	colorless	
Formula weight	289.38 $g \cdot mol^{-1}$	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	**C2/c, (no. 15)**	
Unit cell dimensions	a = 14.0451(4) Å	α= 90°.
	b = 7.1601(7) Å	β= 97.046(6)°.
	c = 28.715(2) Å	γ = 90°.
Volume	2865.9(4) $Å^3$	
Z	8	
Density (calculated)	1.341 $Mg \cdot m^{-3}$	
Absorption coefficient	0.227 mm^{-1}	
F(000)	1232 e	
Crystal size	0.11 x 0.08 x 0.03 mm^3	
θ range for data collection	2.859 to 31.084°.	
Index ranges	$-20 \le h \le 20$, $-10 \le k \le 9$, $-41 \le l \le 41$	
Reflections collected	25294	
Independent reflections	4607 [R_{int} = 0.0485]	
Reflections with I>2σ(I)	3749	
Completeness to θ = 25.242°	99.8 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.99 and 0.98	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4607 / 0 / 182	
Goodness-of-fit on F^2	1.143	
Final R indices [I>2σ(I)]	R_1 = 0.0515	wR^2 = 0.1330
R indices (all data)	R_1 = 0.0683	wR^2 = 0.1496
Largest diff. peak and hole	0.6 and -0.5 e · $Å^{-3}$	

Bond lengths [Å] and angles [°] for 31.

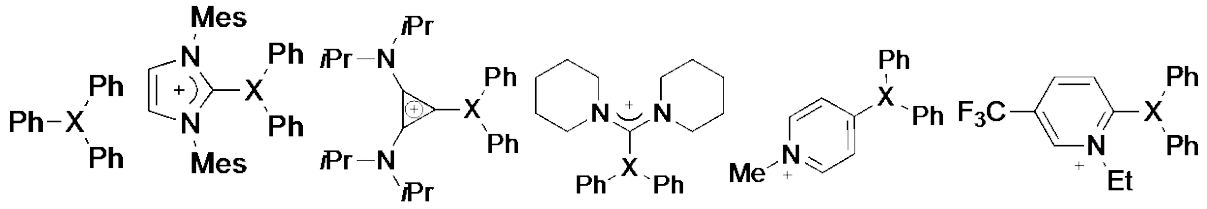
S(1)-O(1)	1.4317(14)	S(1)-O(2)	1.4322(13)
S(1)-N(1)	1.6326(14)	S(1)-C(10)	1.7634(18)
N(1)-C(2)	1.491(2)	N(1)-C(9)	1.417(2)
C(1)-C(2)	1.530(2)	C(1)-C(6)	1.509(2)
C(1)-C(7)	1.507(3)	C(2)-C(3)	1.530(3)
C(3)-C(4)	1.517(3)	C(4)-C(5)	1.534(2)
C(5)-C(6)	1.514(3)	C(6)-C(7)	1.513(3)
C(7)-C(8)	1.473(3)	C(8)-C(9)	1.327(2)
C(10)-C(11)	1.398(2)	C(10)-C(15)	1.386(2)
C(11)-C(12)	1.387(3)	C(12)-C(13)	1.395(3)
C(13)-C(14)	1.391(3)	C(13)-C(16)	1.500(3)
C(14)-C(15)	1.391(3)		

O(1)-S(1)-O(2)	119.68(8)	O(1)-S(1)-N(1)	107.31(8)
O(1)-S(1)-C(10)	107.97(8)	O(2)-S(1)-N(1)	106.75(8)
O(2)-S(1)-C(10)	107.46(8)	N(1)-S(1)-C(10)	107.07(8)
C(2)-N(1)-S(1)	118.71(11)	C(9)-N(1)-S(1)	118.17(11)
C(9)-N(1)-C(2)	120.95(13)	C(6)-C(1)-C(2)	118.33(15)
C(7)-C(1)-C(2)	118.10(14)	C(7)-C(1)-C(6)	60.21(12)
N(1)-C(2)-C(1)	112.25(15)	N(1)-C(2)-C(3)	108.80(15)
C(3)-C(2)-C(1)	112.08(14)	C(4)-C(3)-C(2)	111.32(15)
C(3)-C(4)-C(5)	111.40(15)	C(6)-C(5)-C(4)	114.83(15)
C(1)-C(6)-C(5)	121.22(15)	C(1)-C(6)-C(7)	59.84(12)
C(7)-C(6)-C(5)	125.22(15)	C(1)-C(7)-C(6)	59.95(12)
C(8)-C(7)-C(1)	117.16(15)	C(8)-C(7)-C(6)	125.12(15)
C(9)-C(8)-C(7)	122.26(17)	C(8)-C(9)-N(1)	122.13(16)
C(11)-C(10)-S(1)	118.95(14)	C(15)-C(10)-S(1)	120.68(14)
C(15)-C(10)-C(11)	120.37(17)	C(12)-C(11)-C(10)	119.13(17)
C(11)-C(12)-C(13)	121.48(19)	C(12)-C(13)-C(16)	120.2(2)
C(14)-C(13)-C(12)	118.21(18)	C(14)-C(13)-C(16)	121.6(2)
C(15)-C(14)-C(13)	121.32(18)	C(10)-C(15)-C(14)	119.48(18)

5) Computational details

All geometry optimizations were performed using the Gaussian09 program package. They were carried out using the B3LYP-D3 functional in combination with the def2-TZVP basis set for all atoms except gold and platinum, which were described by the def2-TZVP effective core potential (ECP) and basis set. In order to gain insight into the electronic structure of the complexes, a Natural Bond Orbital (NBO) analysis was performed at the B3LYP-D3/def2-TZVP level using NBO version 3.1 as implemented in the Gaussian09 program package. The analysis of the MO compositions was carried out using AOMix-CDA.

5.1. Ligands: HOMO and LUMO energies and plots



X= As, P

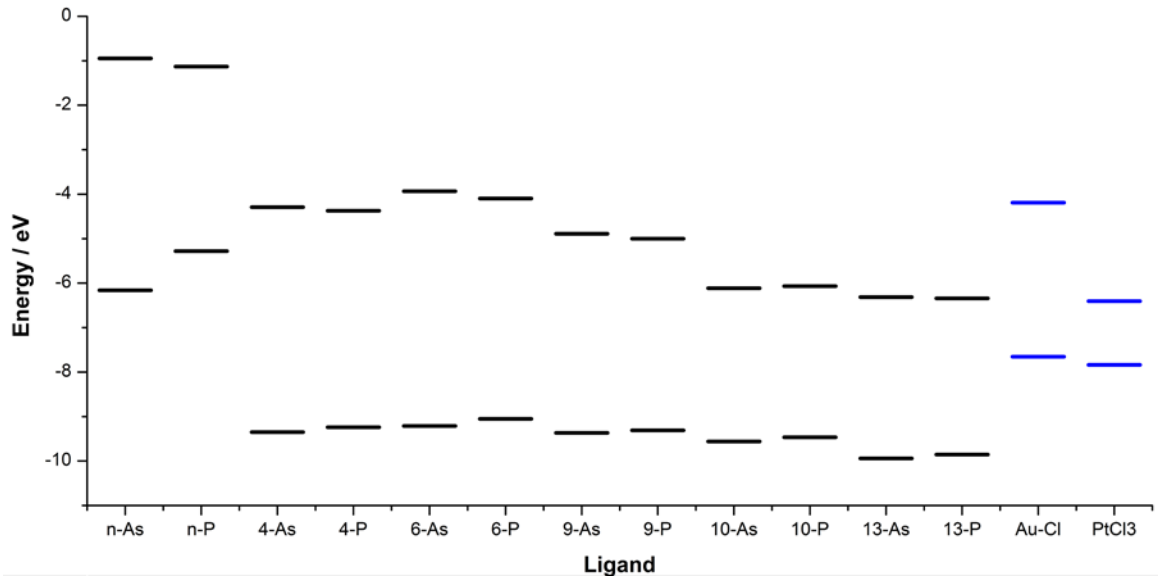
1. Figure S1 presents the HOMO and LUMO energies of all the ligands. The cationic ligands have lower HOMO and LUMO energies than the corresponding neutral analogues.

2. The cationic (and neutral) arsine ligands have lower HOMO and higher LUMO energies than the analogous cationic phosphine ligands.

3. The lower HOMO energies cause the cationic arsine ligands to have slightly poorer electron releasing abilities than the corresponding phosphines. The computational results show that **13-As** has the lowest HOMO energy among all the As ligands.

4. Table 1 shows that the HOMOs of all ligands have lone-pair character at the As/P atom suitable for L→M *σ*-donation, while the LUMOs involve π^*- and σ^*-orbitals that allow for L←M *π*-backdonation, according to the Dewar-Chatt-Duncanson (DCD) model.

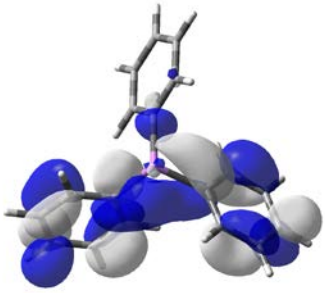
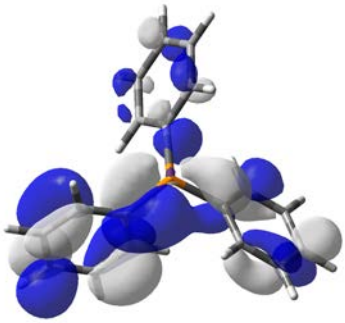
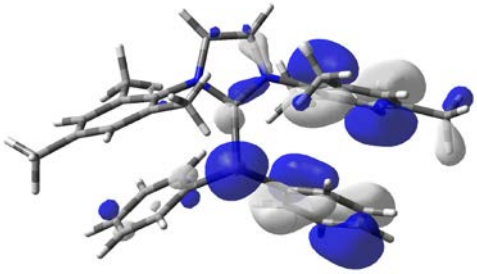
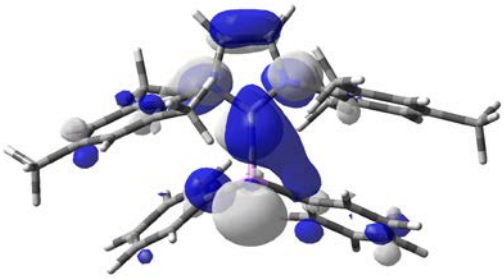
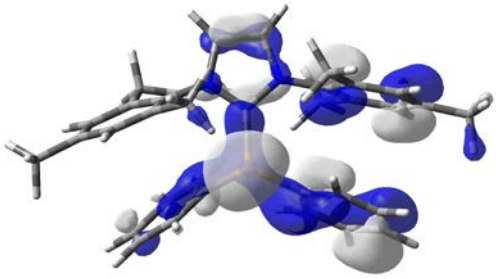
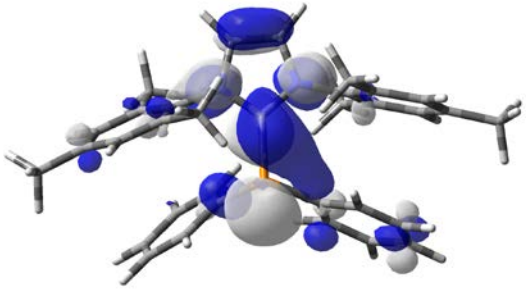
5. Higher-lying *σ* HOMOs and lower-lying π^* LUMOs indicate better electron donors and acceptors, respectively. Hence, the formal substitution of P by an As atom reduces both the *σ*-donor and π-acceptor ability of the ligands. Among all the cationic arsine ligands, the σ donor strength is in the order **6-As** > **3-As** > **9-As** > **10-As** >**13-As**, while the π accepting ability is in the order **13-As** > **10-As** > **9-As** > **3-As** > **6-As**.



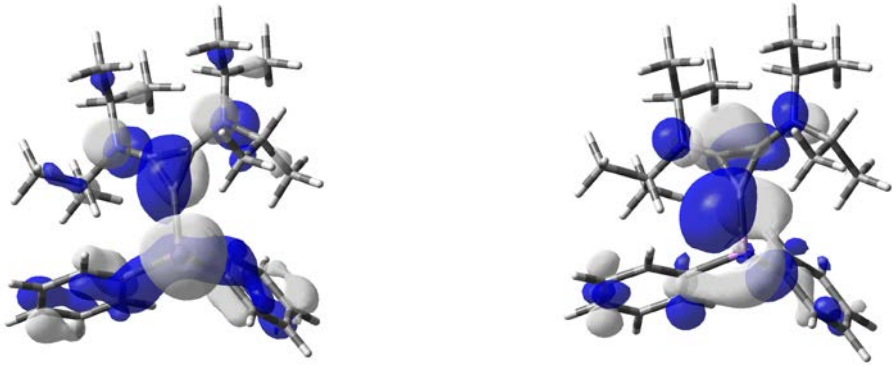
	HOMO	LUMO	HOMO-LUMO gap
n-As	-6.16	-0.95	5.21
n-P	-5.28	-1.13	4.15
3-As	-9.35	-4.29	5.06
3-P	-9.24	-4.37	4.87
6-As	-9.21	-3.93	5.28
6-P	-9.05	-4.10	4.95
9-As	-9.37	-4.89	4.48
9-P	-9.31	-5.00	4.31
10-As	-9.56	-6.11	3.45
10-P	-9.47	-6.07	3.4
13-As	-9.94	-6.31	3.63
13-P	-9.85	-6.34	3.51
AuCl	-7.65	-4.19	3.46
Au	-16.72	-12.29	4.43
$PtCl_3$	-7.55	-6.41	1.14
$PtCl_2$	-1.94	0.30	2.24

Figure S1. HOMO and LUMO energies of all ligands, in eV.

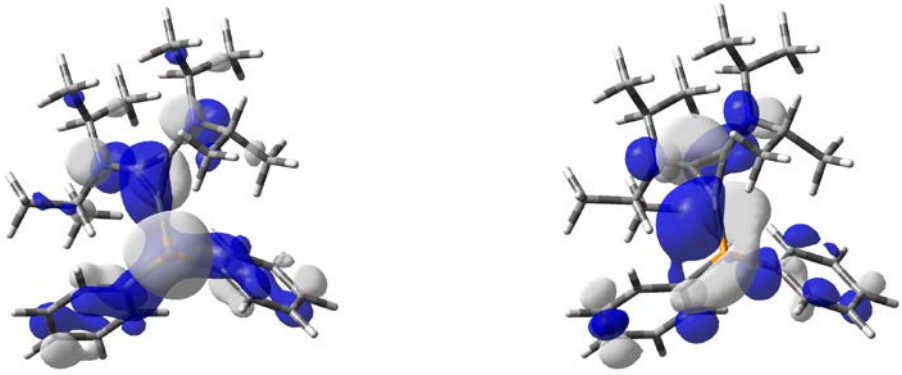
Table S1. Frontier orbitals for all ligands

	HOMO	LUMO
n-As		
n-P		
3-As		
3-P		

6-As

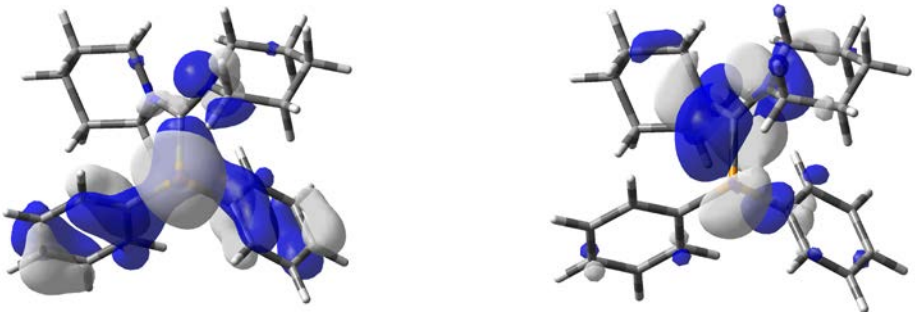


6-P

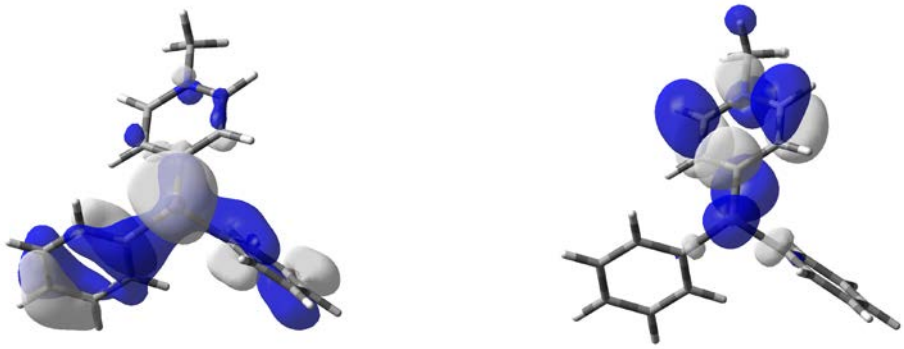


9-As

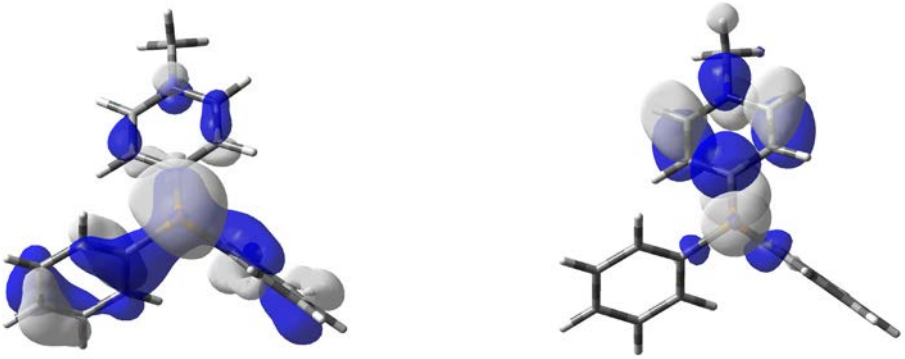
9-P



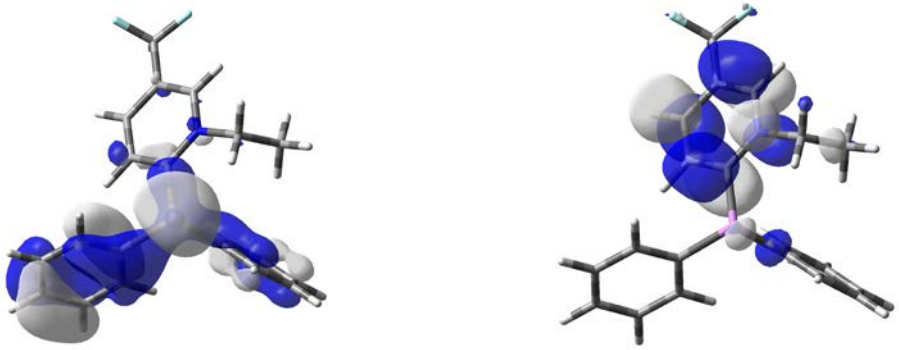
10-As



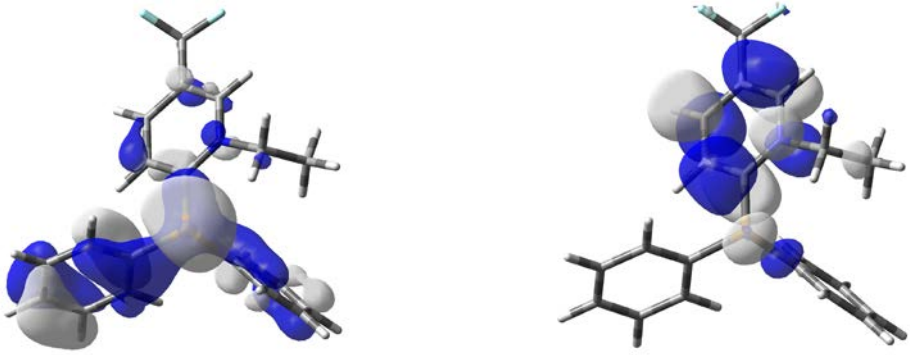
10-P



13-As



13-P



5.2 NBO analysis of cationic arsines/phosphines and their Pt derivatives

1. Table 2 lists the Wiberg bond orders for the bonds between As/P and the three different substituents. The X-C4/C10 bond orders are all very similar; they correspond to the bonds between As/P and the phenyl groups.

2. The bond orders for the X-C1 bond to the cationic substituent are generally smaller than those for the X-C4/C10 bonds to the phenyl groups, except for **10-P**. The higher X-C1 bond order in **10-P** may be correlated with a stronger back donation from P to the pyridine moiety.

3. The X-C1 bond order is smaller in the As ligands than in the corresponding P ligands.

Table S2. Wiberg bond indices for all ligands*

X=As or **P**	**X-C1**	**X-C4**	**X-C10**
n-As		0.8909	
n-P		0.9266	
3-As	0.8432	0.9098	0.9077
3-P	0.9162	0.9410	0.9374
6-As	0.8570	0.8956	0.9023
6-P	0.9189	0.9246	0.9331
9-As	0.8395	0.9094	0.9058
9-P	0.9398	0.9432	0.9435
10-As	0.8934	0.8996	0.9058
10-P	0.9998	0.9331	0.9411
13-As	0.8482	0.9034	0.9081
13-P	0.9286	0.9353	0.9397

*The atomic labels are defined as follows:

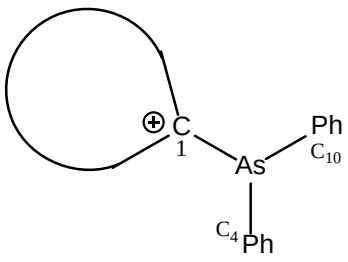


Table S3. Natural bond orbital (NBO) charges for fragments of all ligands*

X=As or **P**	**X**	**R1**	**R2**	**R3**
n-As	0.901	-0.301		
n-P	0.831	-0.277		
3-As	0.939	0.534	-0.231	-0.244
3-P	0.872	0.546	-0.203	-0.215
6-As	0.936	0.569	-0.250	-0.255
6-P	0.870	0.582	-0.222	-0.230
9-As	0.904	0.601	-0.251	-0.253
9-P	0.858	0.584	-0.218	-0.224
10-As	0.973	0.478	-0.238	-0.241
10-P	0.926	0.449	-0.203	-0.209
13-As	0.937	0.523	-0.235	-0.225
13-P	0.871	0.529	-0.203	-0.197

*

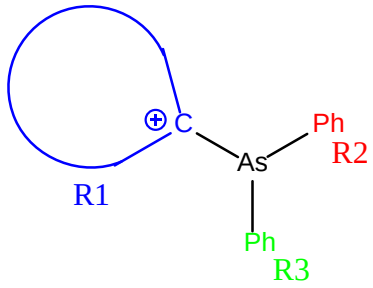
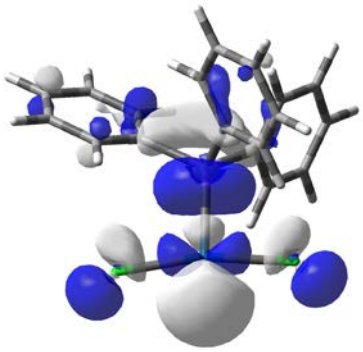
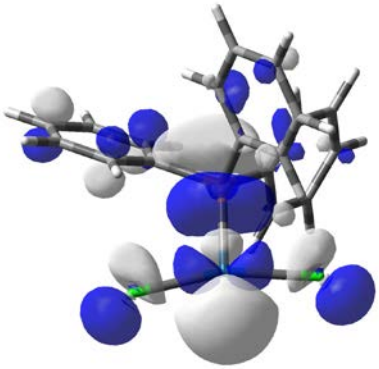
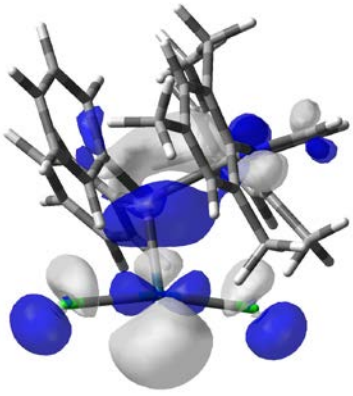
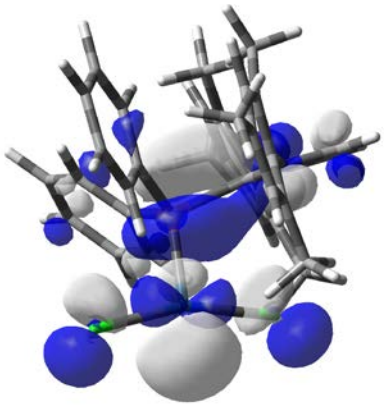
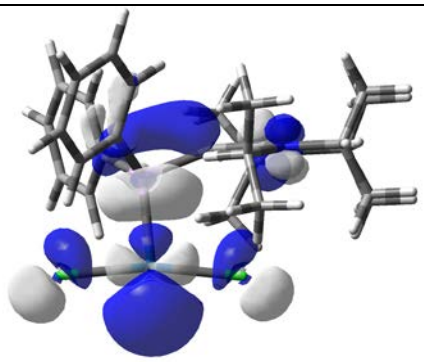
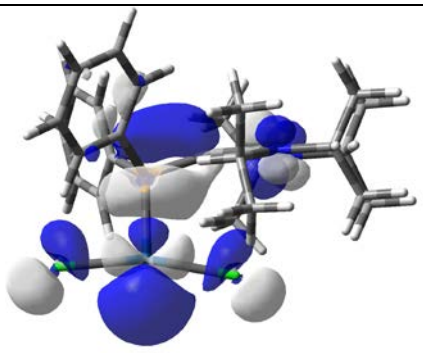


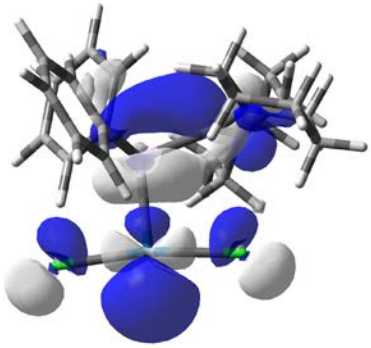
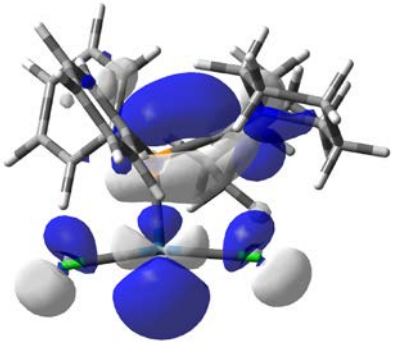
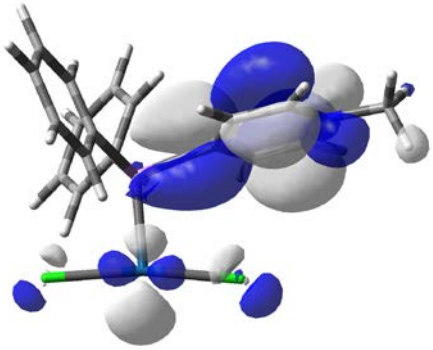
Table S4. Wiberg bond indices for all $PtCl_3$- and $PtCl_2$-species

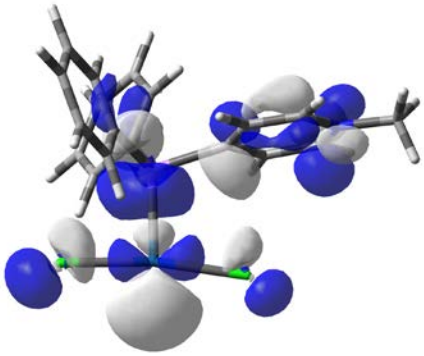
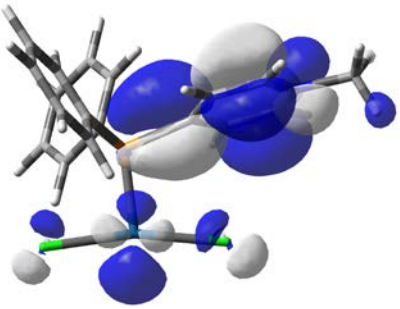
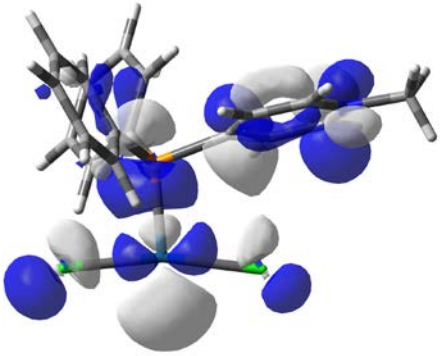
	L-$PtCl_3$				**L-$PtCl_2$**			
X = AS or P	**Pt-X**	**X-C1**	**X-C4**	**X-C10**	**Pt-X**	**X-C1**	**X-C4**	**X-C10**
(n-As)- $PtCl_n$	0.6774	0.8538			0.8832	0.8724		
(n-P)- $PtCl_n$	0.7308	0.8799			0.9322	0.8959		
(3-As)- $PtCl_n$	0.6528	0.7669	0.8762	0.8739	0.8749	0.7862	0.8967	0.8928
(3-P)- $PtCl_n$	0.7003	0.8113	0.8967	0.8948	0.9360	0.8195	0.9217	0.9185
(6-As)- $PtCl_n$	0.6589	0.8095	0.8668	0.8651	0.8724	0.8311	0.8802	0.8798
(6-P)- $PtCl_n$	0.7091	0.8424	0.8887	0.8872	0.9322	0.8599	0.9028	0.9023
(9-As)- $PtCl_n$	0.6581	0.7680	0.8553	0.8682	0.8831	0.7676	0.8780	0.8896
(9-P)- $PtCl_n$	0.7014	0.8116	0.8751	0.8928	0.9339	0.7972	0.8992	0.9166
(10-As)- $PtCl_n$	0.6442	0.8040	0.8639	0.8673	0.8783	0.8121	0.8832	0.8890
(10-P)- $PtCl_n$	0.6932	0.8722	0.8854	0.8874	0.9349	0.8416	0.9062	0.9128
(13-As)- $PtCl_n$	0.6565	0.7768	0.8602	0.8671	0.8835	0.7873	0.8839	0.8907
(13-P)- $PtCl_n$	0.7012	0.8224	0.8856	0.8883	0.9432	0.8145	0.9047	0.9145

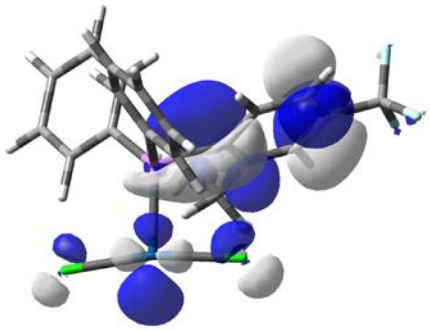
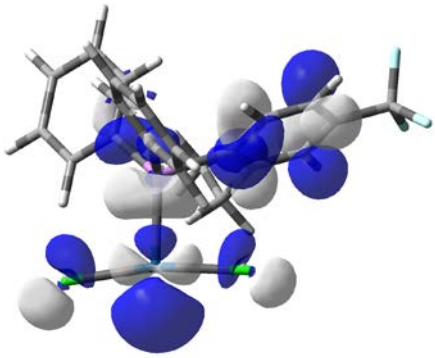
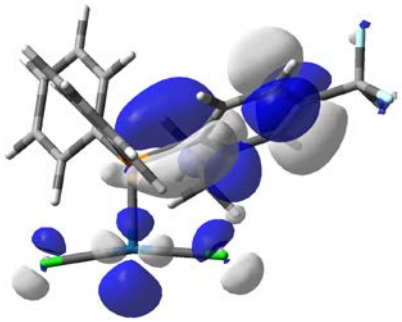
Table S5. Selected molecular orbitals of all $PtCl_2$ coordinated complexes (Fr1: ligand, Fr2: $PtCl_2$)

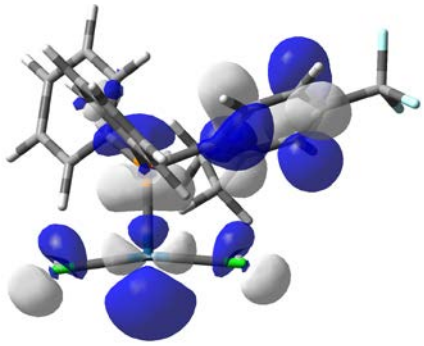
X=As, P	σ^*(X-Pt)-antibond
(Ph_3As)-$PtCl_2$	 LUMO (-3.058 eV) Fr1: 32.4%H, Fr2: 1.1%L+1, 4.3%L+2
(Ph_3P)-$PtCl_2$	 LUMO (-2.973 eV) Fr1: 33.5%H, Fr2: 1.8%L+1, 3.4%L+2
(3-As)-$PtCl_2$	 LUMO (-6.086 eV) Fr1: 28.4%H, Fr2: 1.9%L+2

(3-P)-$PtCl_2$	 LUMO (-6.041 eV) Fr1: 28.9%H, Fr2: 1.2%L
(6-As)-$PtCl_2$	 LUMO (-5.986 eV) Fr1: 28.7%H, Fr2: 2.5%L+2
(6-P)-$PtCl_2$	 LUMO (-5.939 eV) Fr1: 29.9%H, Fr2: 1.9%L+2

(9-As)-$PtCl_2$	 LUMO (-6.218 eV) Fr1: 28.7%H, Fr2: 2.3%L+2
(9-P)-$PtCl_2$	 LUMO (-6.289 eV) Fr1: 28.7%H, Fr2: 2.3%L+2
(10-As)-$PtCl_2$	 LUMO (-6.633 eV) Fr1: 63.1%L, Fr2: 11.0%H-3

	 LUMO+1 (-5.642 eV) Fr1: 32.6%L, 13.1%H, Fr2: 30.2%H-3, 1.1%L+1, 3.2%L+2
(10-P)-$PtCl_2$	 LUMO (-6.713 eV) Fr1: 57.6%L, Fr2: 11.7%H-3  LUMO+1 (-5.514 eV) Fr1: 34.3%L, 10.3%H, Fr2: 25.7%H-3, 2.0%L+1, 2.3%L+2

(13-As)-$PtCl_2$	 LUMO (-6.726 eV) Fr1: 59.7%L, Fr2: 13.8%H-3  LUMO+1 (-6.229 eV) Fr1: 38.6%L, 12.9%H, Fr2: 27.3%H-3, 2.1%L+2
(13-P)-$PtCl_2$	 LUMO (-6.831 eV) Fr1: 36.3%L, Fr2: 12.0%H

	 LUMO+1 (-6.109 eV) Fr1: 38.6%L, 12.9%H, Fr2: 23.7%H-3, 1.6%L+2

5.3. Evaluation of CEPs and TEPs for arsine ligands

All calculations were performed with the Gaussian09 software package. The complex $LNi(CO)_3$ was optimized using the B3LYP-D3 functional with the LanL2DZ effective core potential for Ni and the def2-TZVP basis set for all other atoms. Each local minimum was verified by an analytical frequency calculation. The *v*(CO) (A_1) vibrational frequency (without any scaling) defines the computed electronic parameter (CEP). The CEPs provide information about the net donor/acceptor character of the ligands L, according to Tolman's proposal.

Table S6. Computed CEP (cm^{-1}) and experimental TEP (cm^{-1}) for selected ligands.

Ligand	CEP	TEP
PH_3	2153.6	2083.2[a]
AsH_3	2153.0	2080.6[a]
PMe_3	2133.8	2064.1[a]
$AsMe_3$	2138.1	2067.0[a]
PF_3	2175.6	2110.8[a]
AsF_3	2184.8	2114.7[a]
PPh_3	2136.1	2068.9[b]
$AsPh_3$	2140.3	2071.7, 2071.9
$As(PhF)_3$	2143.7	2075.8
$As(PhCl)_3$	2144.1	2076.6
P^tBu_3	2125.0	2056.1[b]
$P(OEt)_3$	2144.6	2076.3[b]
$As(PhPr)_3$	2135.1	2064.9

Experimental TEP from: [a] *Inorg. Chem*. 2001, 40, 5806. [b] Tolman, C. A. *Chem. Rev.* 1977, 77, 313.

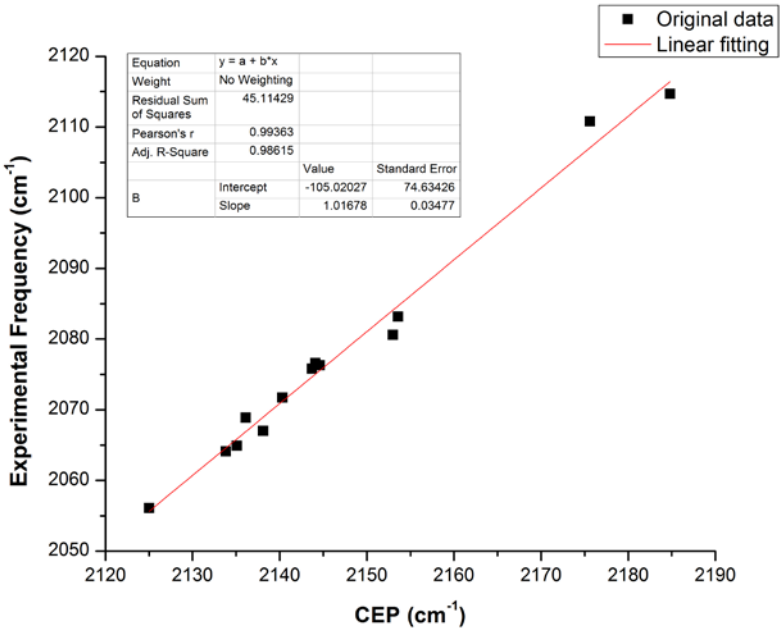


Figure S2. Correlation between CEP (cm^{-1}) and TEP (cm^{-1}).

We obtain a good correlation between CEP and the Tolman Electronic Parameter (TEP) :

(1) TEP = 1.0168 CEP – 105.0 cm^{-1} (R^2 = 0.9862)

This relation can be used to estimate the TEP for other PL_3 or AsL_3 ligands that are not available experimentally.

The cone angles were computed from the optimized geometries (Table S7).

Table S7. Computed CEP (cm^{-1}), predicted TEP (cm^{-1}) using equation 1, and cone angle (deg) determined from the DFT optimized geometries.

Ligand	CEP	Predicted TEP	Cone angle
PH_3	2153.6	2084.8	87
AsH_3	2153.0	2084.2	84
PMe_3	2133.8	2064.6	119
$AsMe_3$	2138.1	2069.0	114
PF_3	2175.6	2107.2	104
AsF_3	2184.8	2116.5	99
PPh_3	2136.1	2067.0	148

$AsPh_3$	2140.3	2071.3	144
$As(PhF)_3$	2143.7	2074.7	149
$As(PhCl)_3$	2144.1	2075.1	148
P^tBu_3	2125.0	2055.7	182
As^tBu_3	2126.8	2057.5	89
$P(OEt)_3$	2144.6	2075.6	130
$As(OEt)_3$	2161.3	2092.6	125
$P(PhMe)_3$	2133.3	2064.1	163
$As(PhMe)_3$	2138.4	2069.3	160
$As(PhPr)_3$	2135.1	2066.0	217
3-P	2157.9	2089.2	172
3-As	2161.3	2092.6	178
6-P	2153.1	2084.3	157
6-As	2156.2	2087.4	154
9-P	2159.6	2090.9	160
9-As	2160.9	2092.2	156
10-P	2156.2	2087.4	155
10-As	2160.0	2091.3	150
13-P	2163.1	2094.4	150
13-As	2165.6	2097.0	144

5.4. Free energy profile for the cyclization of 30 to 31 using arsine ligands

Density functional theory (DFT) was employed to explore the reaction mechanism. Geometries were optimized using the B3LYP-D3[18,19] functional with the def2-SVP[20] effective core potential for Pt and the SVP basis set for all other atoms. The same level of theory was used for frequency calculations to confirm each stationary point to be either a minimum or transition state (TS) structure. Single-point calculations, in which the SVP basis set was replaced by the larger TZVP[21] basis, at the gas-phase optimized geometries were carried out with inclusion of continuum solvation.[22] All calculations were carried out with the Gaussian09 program package.[23]

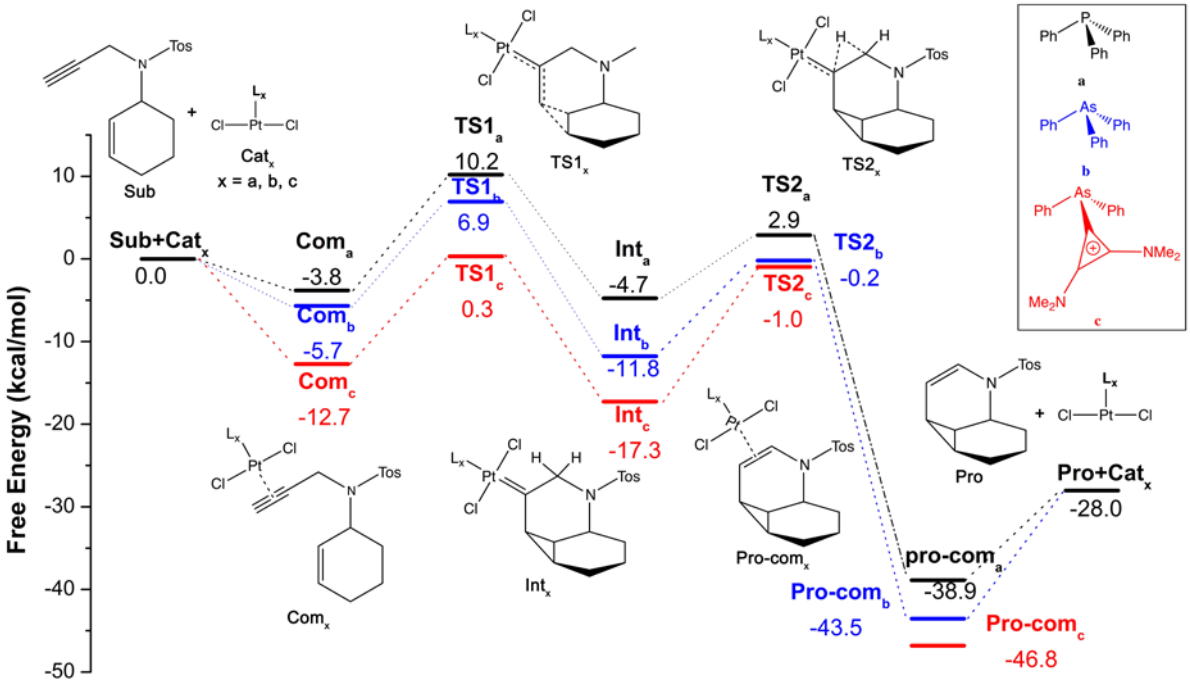


Figure S3. Free energy profiles (kcal/mol) in CH_2Cl_2 solution for the cyclization of **30** (**Sub**) to **31** (**Pro**).

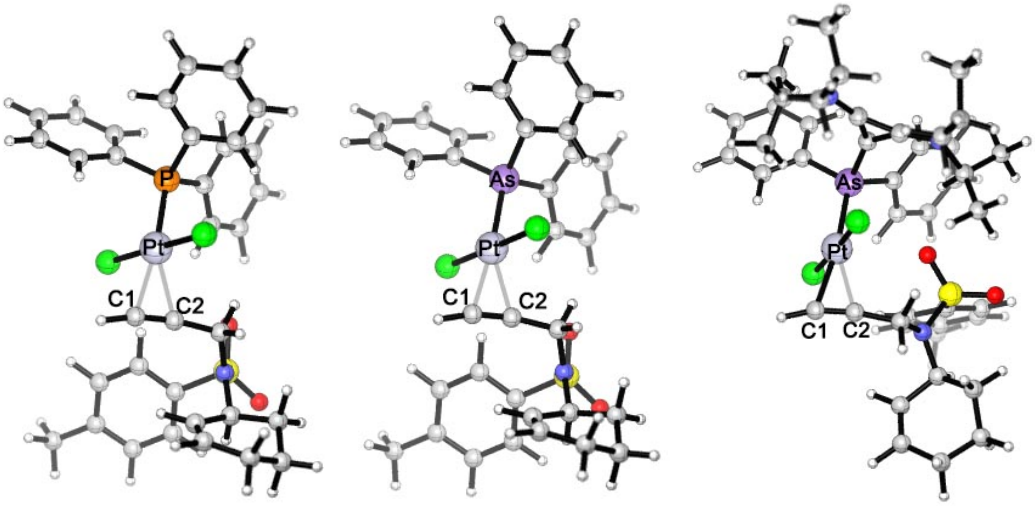


Figure S4. Optimized geometries of **Com$_a$** (left): Pt−C1: 2.28 Å, Pt−C2: 2.29 Å; **Com$_b$** (middle): Pt−C1: 2.24 Å, Pt−C2: 2.24 Å; **Com$_c$** (right): Pt−C1: 2.21 Å, Pt−C2: 2.24 Å.

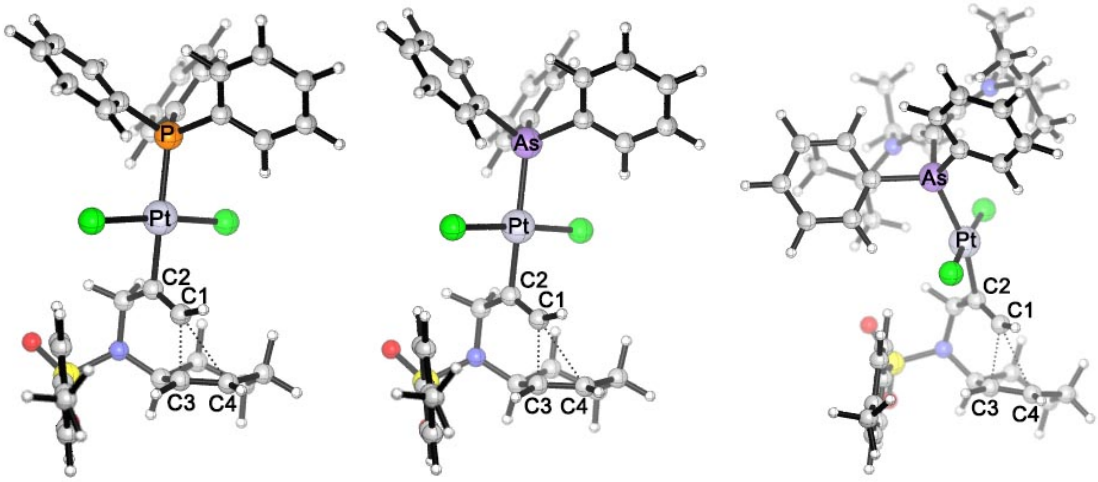


Figure S5. Optimized geometries of **TS1$_a$** (left): C1−C3: 1.96 Å, C1−C4: 2.39 Å; **TS1$_b$** (middle): C1−C3: 1.98 Å, C1−C4: 2.39 Å; **TS1$_c$** (right): C1−C3: 2.15 Å, C1−C4: 2.45 Å.

Energies for all computed species

Table S8. Zero-point vibrational energy corrections (*ZPVE*), enthalpy corrections (H_{corr}), and Gibbs free energy corrections (G_{corr}) evaluated on the gas-phase geometries at the B3LYP-D3/def2-SVP level, and single-point solvent-corrected SCF energies (*E*) at the B3LYP-D3/def2-TZVP level. All energies are in atomic units.

	ZPVE	H_{corr}	G_{corr}	***E***
		Pathway a		
Sub+Cat$_a$	0.598288	0.641057	0.492533	-3299.255965
Com$_a$	0.598877	0.640682	0.519028	-3299.288548
TS1$_a$	0.59955	0.640837	0.520185	-3299.267362
Int$_a$	0.602836	0.6416	0.528676	-3299.29967
TS2$_a$	0.599225	0.638629	0.523252	-3299.282088
Pro-com$_a$	0.606117	0.645641	0.53384	-3299.359232
Pro+Cat$_a$	0.602718	0.643623	0.497644	-3299.305747

Pathway b				
Sub+Cat$_b$	0.596212	0.63975	0.48861	-5193.611829
Com$_b$	0.596966	0.639473	0.515624	-5193.647892
TS1$_b$	0.59758	0.639653	0.515861	-5193.628016
Int$_b$	0.601674	0.641623	0.526847	-5193.668819
TS2$_b$	0.596671	0.636124	0.518988	-5193.642514
Pro-com$_b$	0.603557	0.645008	0.526106	-5193.718695
Pro+Cat$_b$	0.600642	0.642316	0.493721	-5193.66161
Pathway c				
Sub+Cat$_c$	0.916107	0.976645	0.791286	-5659.46358
Com$_c$	0.917991	0.977774	0.821798	-5659.514364
TS1$_c$	0.91752	0.9757	0.822159	-5659.481203
Int$_c$	0.922151	0.980107	0.826555	-5659.526357
TS2$_c$	0.916798	0.973106	0.824819	-5659.498638
Pro-com$_c$	0.923234	0.982048	0.824834	-5659.571681
Pro+Cat$_c$	0.920537	0.979211	0.796397	-5659.513361

Table S9. Relative energies with ZPVE correction (*E*), enthalpies (*H*), and Gibbs free energies (*G*) in CH_2Cl_2 solution at the B3LYP-D3/def2-TZVP//B3LYP-D3/def2-SVP level. All energies are in kcal/mol.

	E	**H**	**G**
		Pathway a	
Sub+Cat$_a$	0	0	0
Com$_a$	-20.1	-20.7	-3.8
TS1$_a$	-6.4	-7.3	10.2
Int$_a$	-24.6	-27.1	-4.7
TS2$_a$	-15.8	-17.9	2.9
Pro-com$_a$	-59.9	-61.9	-38.9
Pro+Cat$_a$	-28.5	-29.6	-28.0
		Pathway b	
Sub+Cat$_b$	0	0	0
Com$_b$	-22.2	-22.8	-5.7
TS1$_b$	-9.3	-10.2	6.9
Int$_b$	-32.3	-34.6	-11.8
TS2$_b$	-19.0	-21.5	-0.2
Pro-com$_b$	-62.5	-63.8	-43.5
Pro+Cat$_b$	-28.5	-29.6	-28.0
		Pathway c	
Sub+Cat$_c$	0	0	0
Com$_c$	-30.7	-31.2	-12.7
TS1$_c$	-10.2	-11.7	0.3

Int_c	-35.6	-37.2	-17.3
$TS2_c$	-21.6	-24.2	-1.0
$Pro\text{-}com_c$	-63.4	-64.4	-46.8
$Pro+Cat_c$	-28.5	-29.6	-28.0

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5.5.- Cartesian coordinates (Å) for all computed species and imaginary frequencies for all transition states

SUB:

C	1.43942200	-0.86011400	-1.06648300
C	1.97326300	-1.52818900	0.14493000
C	1.16443700	-0.35611900	-2.15699600
N	3.26391000	-1.03730400	0.58167700
H	2.03897400	-2.60645200	-0.06755000
H	1.25144300	-1.41246300	0.96164800
H	1.14445800	0.07484800	-3.14280500
S	3.35551300	0.15350800	1.75706200
C	3.84319900	1.62127100	0.86929100
O	4.45263200	-0.19647900	2.66333300
O	1.98627100	0.33622400	2.25369500
C	5.15581100	2.08301600	0.96699600
C	2.90109500	2.26613800	0.06303800
C	5.53164100	3.20594300	0.22567900
H	5.86100900	1.57063400	1.62265000
C	3.29612500	3.38219200	-0.66738400
H	1.86903400	1.91848500	-0.00068500
C	4.61417100	3.86946200	-0.60217500
H	6.55803700	3.57508000	0.29563500
H	2.55631400	3.88248600	-1.29793200
C	5.01513300	5.08554300	-1.39583000
H	4.47763300	5.98101300	-1.04149300
H	6.09330800	5.28577900	-1.31675700
H	4.76561200	4.96369500	-2.46227100
C	4.51558200	-1.62362700	0.07942800
C	4.78468700	-2.99860200	0.70550600
C	4.52440400	-1.66539300	-1.42992700
H	5.31492900	-0.93610300	0.40348500
C	5.91285000	-3.72475200	-0.02666500
H	3.86415200	-3.60472300	0.64216500
H	5.00542500	-2.85790300	1.77356100
C	4.97403100	-2.71242500	-2.13245400
C	5.55169700	-3.95130500	-1.49942100
H	6.13748700	-4.68332200	0.46705500
H	6.83374600	-3.11770600	0.03129900
H	6.43732700	-4.27904600	-2.07028300
H	4.82278700	-4.77987600	-1.59094500
H	4.14606900	-0.77537700	-1.94006100
H	4.93566200	-2.67532700	-3.22647800

PPh_3-$PtCl_2$:

P	0.36953800	-0.09545100	0.00835800
C	1.57471000	1.18826300	-0.46247800
C	2.40731700	1.01534200	-1.57753200
H	2.32732800	0.11695300	-2.18998900
C	3.34669000	1.99732700	-1.90515200
H	3.99081900	1.85832900	-2.77624300
C	2.62656500	3.32294800	-0.01155300
H	2.70458200	4.22723900	0.59582900
C	0.89864100	-0.69840900	1.64812500
C	0.04814500	-1.55111500	2.37250400
H	-0.93414200	-1.80683200	1.96937000
C	0.46948200	-2.07163800	3.59608600
H	-0.19587800	-2.73241800	4.15621600
C	1.73031600	-1.74627800	4.10664900
H	2.05230800	-2.15155800	5.06886500
C	2.57711000	-0.90034400	3.38643600
H	3.56346400	-0.64412400	3.77984800
C	2.16641500	-0.37503400	2.15883200
H	2.83531500	0.28118700	1.60147700
C	0.64823500	-1.47009100	-1.15493500
C	1.58680700	-2.46843700	-0.85895000
H	2.11402400	-2.46178800	0.09654500
C	1.84160200	-3.47860800	-1.78969700
H	2.56789700	-4.25988400	-1.55446800
C	1.16601900	-3.49216800	-3.01258800
H	1.36437300	-4.28569500	-3.73688400
C	0.22898200	-2.49586600	-3.30649300
H	-0.30790100	-2.51050200	-4.25746900
C	-0.03553300	-1.48805000	-2.37983700
H	-0.78136000	-0.72033900	-2.59443600
C	1.68250800	2.35293200	0.31699000
H	1.01596000	2.50682200	1.16574600
C	3.45886000	3.14821200	-1.12338600
H	4.19231600	3.91552400	-1.38215700
Pt	-1.71941500	0.56591100	0.00073900
Cl	-1.48657500	2.86347100	-0.04711600
Cl	-2.54136700	-1.61500700	0.03868400

$AsPh_3$-$PtCl_2$:

As	0.35470700	-0.02204300	-0.00469900
C	1.43514400	1.50336500	-0.50415400
C	2.40788100	1.36767900	-1.50257400
H	2.52713100	0.42272000	-2.03504000
C	3.23059500	2.45381200	-1.81639800
H	3.98764300	2.35035900	-2.59711200
C	2.10468700	3.79628100	-0.14358800
H	1.97880200	4.74635700	0.38035800
C	1.04294700	-0.57457000	1.71782900
C	0.36907800	-1.57234100	2.43644600
H	-0.55729900	-1.99746300	2.04200100
C	0.89618300	-2.01322900	3.65152400
H	0.37385600	-2.79019900	4.21434000
C	2.08130600	-1.46128600	4.14932900
H	2.48631200	-1.80733600	5.10329800
C	2.74602100	-0.46418100	3.43078300
H	3.67027700	-0.02984600	3.81888400
C	2.22920800	-0.01530200	2.21205800
H	2.74960400	0.76426800	1.65326600
C	0.86766300	-1.41958000	-1.23546600
C	1.97801400	-2.22323500	-0.95174200
H	2.52768000	-2.09627600	-0.01670000
C	2.37426400	-3.19788100	-1.87180900
H	3.23709100	-3.83102900	-1.65257600
C	1.66427100	-3.36541700	-3.06391700
H	1.97362100	-4.13092300	-3.77940500
C	0.55322600	-2.56149100	-3.33932400
H	-0.00787100	-2.69927700	-4.26623500
C	0.14855400	-1.58811700	-2.42464200
H	-0.73054900	-0.97174900	-2.62321200
C	1.27526200	2.72031300	0.17327100
H	0.48968100	2.83571100	0.92070600
C	3.08176600	3.66465400	-1.13650000
H	3.72431400	4.51262200	-1.38508900
Pt	-1.91939300	0.31328300	0.01408800
Cl	-2.03082100	2.61668800	-0.12429600
Cl	-2.28326200	-1.98629900	0.15912000

Com_a:

C	-3.67856700	1.48003800	-0.54246200
C	-4.32837800	2.39548900	0.29331900
H	-4.26921800	2.28707500	1.37713100
C	-5.04269100	3.46025400	-0.26306800
H	-5.54191100	4.17728400	0.39281300

C	-5.11373000	3.61082800	-1.64983000
H	-5.67166600	4.44530200	-2.08131500
C	-4.46022100	2.69923100	-2.48596900
H	-4.50243100	2.82093600	-3.57072100
C	-3.73778800	1.64134100	-1.93544600
H	-3.20288100	0.94263400	-2.58284000
C	-2.46787900	0.32610200	1.89301500
C	-1.18592700	0.68787800	2.33292600
H	-0.36624700	0.80292400	1.62614800
C	-0.94456600	0.89079100	3.69344400
H	0.06856100	1.14256900	4.01219500
C	-1.98168200	0.74978500	4.61801100
H	-1.79168000	0.90704300	5.68264900
C	-3.26364200	0.39304100	4.18374200
H	-4.07497400	0.27376200	4.90578800
C	-3.50742600	0.17228100	2.82768000
H	-4.50187200	-0.13330500	2.49645000
Pt	-0.77590400	-0.30599200	-0.95424700
Cl	-0.44473200	2.03759800	-0.89757600
Cl	-1.07424600	-2.63230000	-1.07006300
C	1.43942200	-0.86011400	-1.06648300
C	1.97326300	-1.52818900	0.14493000
C	1.16443700	-0.35611900	-2.15699600
N	3.26391000	-1.03730400	0.58167700
H	2.03897400	-2.60645200	-0.06755000
H	1.25144300	-1.41246300	0.96164800
H	1.14445800	0.07484800	-3.14280500
S	3.35551300	0.15350800	1.75706200
C	3.84319900	1.62127100	0.86929100
O	4.45263200	-0.19647900	2.66333300
O	1.98627100	0.33622400	2.25369500
C	5.15581100	2.08301600	0.96699600
C	2.90109500	2.26613800	0.06303800
C	5.53164100	3.20594300	0.22567900
H	5.86100900	1.57063400	1.62265000
C	3.29612500	3.38219200	-0.66738400
H	1.86903400	1.91848500	-0.00068500
C	4.61417100	3.86946200	-0.60217500
H	6.55803700	3.57508000	0.29563500
H	2.55631400	3.88248600	-1.29793200
C	5.01513300	5.08554300	-1.39583000
H	4.47763300	5.98101300	-1.04149300
H	6.09330800	5.28577900	-1.31675700
H	4.76561200	4.96369500	-2.46227100
C	4.51558200	-1.62362700	0.07942800
C	4.78468700	-2.99860200	0.70550600
C	4.52440400	-1.66539300	-1.42992700
H	5.31492900	-0.93610300	0.40348500
C	5.91285000	-3.72475200	-0.02666500
H	3.86415200	-3.60472300	0.64216500
H	5.00542500	-2.85790300	1.77356100
C	4.97403100	-2.71242500	-2.13245400
C	5.55169700	-3.95130500	-1.49942100
H	6.13748700	-4.68332200	0.46705500
H	6.83374600	-3.11770600	0.03129900
H	6.43732700	-4.27904600	-2.07028300
H	4.82278700	-4.77987600	-1.59094500
H	4.14606900	-0.77537700	-1.94006100
H	4.93566200	-2.67532700	-3.22647800
C	-4.00358200	-1.31963000	0.09673200
C	-5.20907700	-1.21456500	-0.61019100
C	-3.71303100	-2.49905900	0.80309100
C	-6.11765300	-2.27709900	-0.60630400
H	-5.44627200	-0.30314700	-1.16007000
C	-4.62558900	-3.55206500	0.80868100
H	-2.77051700	-2.59115600	1.34316700
C	-5.82881200	-3.44445800	0.10273300
H	-7.05625600	-2.18656400	-1.15797700
H	-4.39284200	-4.46554400	1.36057200
H	-6.54085600	-4.27325700	0.10610400
P	-2.77865400	0.03565000	0.11626500

Com$_b$:

As	-2.69143000	0.01393300	0.06180700
C	-3.64389000	1.61918500	-0.44979400
C	-4.32714700	2.39159600	0.49511900
H	-4.29424000	2.12426900	1.55311800
C	-5.04437100	3.51756100	0.08033000
H	-5.57307300	4.12504100	0.81868200
C	-5.08068500	3.86740200	-1.27208100
H	-5.64077300	4.74891000	-1.59320700
C	-4.39289800	3.09532800	-2.21398800
H	-4.41095300	3.37337200	-3.27031200
C	-3.66914700	1.97434500	-1.80445000
H	-3.11099900	1.38335000	-2.53425700
C	-2.34455000	0.15462400	1.96276700
C	-1.06330600	0.52165500	2.39546400
H	-0.27147400	0.73937900	1.67902600
C	-0.78789400	0.59864700	3.76273700
H	0.22416500	0.85804300	4.07879700
C	-1.79202900	0.32445500	4.69509800
H	-1.57556000	0.38267300	5.76468600
C	-3.07268000	-0.03748100	4.26260500
H	-3.85602800	-0.25946300	4.99143000
C	-3.35125400	-0.13175600	2.89696500
H	-4.34395100	-0.44097400	2.56244800
Pt	-0.57483600	-0.28645700	-1.04525100
Cl	-0.28106300	2.05434700	-0.88736300
Cl	-0.89402800	-2.60785700	-1.21657900
C	1.60355100	-0.81671900	-1.05166200
C	2.11164900	-1.49750100	0.16518200
C	1.37509400	-0.31135800	-2.15663900
N	3.40680800	-1.03703400	0.61946000
H	2.15542100	-2.57649900	-0.05024200
H	1.38422300	-1.36777700	0.97484600
H	1.42983400	0.11476100	-3.14394300
S	3.50847200	0.15190900	1.79650700
C	3.99755600	1.62038200	0.91066300
O	4.60869900	-0.20670900	2.69525800
O	2.14241200	0.33935200	2.29969000
C	5.31654500	2.06745400	0.98998700
C	3.05093300	2.27823400	0.12041600
C	5.69364300	3.18832300	0.24628600
H	6.02586400	1.54581400	1.63380100
C	3.44744400	3.39141100	-0.61362000
H	2.01473300	1.94145200	0.07091700
C	4.77152200	3.86401900	-0.56653800
H	6.72490300	3.54612100	0.30219500
H	2.70410800	3.90064200	-1.23273800
C	5.17410900	5.07802800	-1.36252300
H	4.65740800	5.97947800	-0.99266700
H	6.25651200	5.26203000	-1.30463900
H	4.90082200	4.96551300	-2.42411400
C	4.65289500	-1.62854900	0.10925200
C	4.89458700	-3.02419600	0.69982700
C	4.67442700	-1.62894400	-1.40054400
H	5.45999000	-0.96367600	0.45964400
C	6.01546700	-3.74933100	-0.04450400
H	3.96480700	-3.61312500	0.61451800
H	5.11048900	-2.91588000	1.77268800
C	5.11071000	-2.66426700	-2.12836200
C	5.66023000	-3.93042700	-1.52497700
H	6.22113100	-4.72426400	0.42481300
H	6.94565400	-3.15917400	0.03488100

H	6.54352900	-4.25967300	-2.09855100
H	4.91655100	-4.74232400	-1.64312400
H	4.31813100	-0.71766100	-1.88849700
H	5.08261900	-2.59625500	-3.22121200
C	-4.05791700	-1.35829800	-0.03573800
C	-5.31101600	-1.08453900	-0.59738000
C	-3.78080400	-2.63331400	0.47962700
C	-6.28771000	-2.08450600	-0.63949700
H	-5.53128400	-0.09307700	-0.99672100
C	-4.76215200	-3.62413600	0.43862800
H	-2.79862700	-2.85401800	0.89833000
C	-6.01518600	-3.35225700	-0.12091300
H	-7.26515700	-1.86763000	-1.07690400
H	-4.54446400	-4.61656800	0.84008900
H	-6.77983800	-4.13215500	-0.15321000

Com$_c$:

As	-1.24182200	0.81951600	-0.88638100
N	-4.41437900	-1.36371200	-0.04229100
N	-3.20543600	0.68025400	2.87040900
C	-2.70187900	0.51945400	0.33283900
C	-3.70415800	-0.41426200	0.51547900
C	-3.22957200	0.36143900	1.59992000
C	-5.40150400	-2.17747200	0.70971900
H	-5.81967200	-2.86206100	-0.03984100
C	-6.55263400	-1.31106000	1.21892000
H	-6.21060300	-0.53640000	1.92094300
H	-7.29349600	-1.93301100	1.74263200
H	-7.05715500	-0.80550000	0.38250800
C	-4.71748800	-3.03141500	1.77725000
H	-3.92835300	-3.65236600	1.33231200
H	-5.45356900	-3.68995300	2.26198400
H	-4.24676800	-2.41836000	2.55697200
C	-4.13561300	-1.70960800	-1.46615500
H	-3.34992800	-1.01380200	-1.78001600
C	-5.36037900	-1.44893600	-2.33910700
H	-6.19293900	-2.12817000	-2.09804700
H	-5.09828300	-1.60734200	-3.39552100
H	-5.70785800	-0.41151800	-2.22984500
C	-3.57768900	-3.12524200	-1.59475100
H	-2.70155200	-3.25190800	-0.94384900
H	-3.26888000	-3.29644900	-2.63692100
H	-4.32687200	-3.89223500	-1.34448300
C	-4.11546200	0.03365700	3.84515600
H	-4.76035200	-0.61487300	3.24226700
C	-5.00747300	1.06269700	4.53746200
H	-5.73315700	0.54709300	5.18386600
H	-5.56604200	1.66150300	3.80227200
H	-4.42959500	1.74863400	5.17507300
C	-3.33819700	-0.85188700	4.81846900
H	-2.69256300	-0.26073800	5.48523800
H	-2.70599000	-1.56986500	4.27539800
H	-4.04185400	-1.41368100	5.45065500
C	-2.15782700	1.62019100	3.36949800
H	-2.39931300	1.76489800	4.43095500
C	-2.27393200	2.97800000	2.68034000
H	-1.54001200	3.67490700	3.10975800
H	-3.27907000	3.40378400	2.81912600
H	-2.06459000	2.91475800	1.60469900
C	-0.77803500	0.97770000	3.26894900
H	-0.54089200	0.66453600	2.24712700
H	-0.70689600	0.07939400	3.89640700
H	0.00264200	1.68173400	3.58748900
C	-2.26527900	1.13905200	-2.50116800
C	-3.50768000	1.78818500	-2.41419500
H	-3.89668300	2.11557500	-1.44730500
C	-4.25775400	2.00778800	-3.57078700
H	-5.22336000	2.51395200	-3.50327400
C	-3.77397100	1.57839000	-4.81101300
H	-4.36430400	1.74747400	-5.71428400
C	-2.53578500	0.93633300	-4.89414500
H	-2.15423400	0.60460000	-5.86222300
C	-1.77415000	0.71519900	-3.74264000
H	-0.80084300	0.22594800	-3.80846600
C	-0.44632300	2.51012500	-0.40522900
C	0.60838000	2.50773200	0.51390900
H	0.98913200	1.57517400	0.93061200
C	1.17929100	3.72113700	0.90374300
H	2.01039200	3.71766700	1.61136500
C	0.70615100	4.92272200	0.37171900
H	1.15846100	5.86981200	0.67486500
C	-0.33769600	4.91662600	-0.56075500
H	-0.69869100	5.85518700	-0.98703000
C	-0.91770100	3.70966900	-0.95681200
H	-1.72309100	3.70911300	-1.69291100
Pt	0.16879400	-1.13854200	-0.82809400
Cl	1.38901900	-0.20208600	-2.61656400
Cl	-1.01400900	-2.11906000	0.96689100
C	1.79349700	-2.64951100	-0.32008200
C	2.60374800	-2.44926500	0.89141200
C	1.18291500	-3.04040200	-1.32150300
N	3.55269800	-1.34962800	0.78945600
H	3.13100700	-3.39652300	1.09290800
H	1.91273200	-2.27342700	1.72837400
H	0.86555900	-3.57382600	-2.20331600
S	3.34849200	-0.07846600	1.86821900
C	3.90985600	1.32685500	0.92642600
O	4.21091800	-0.20129700	3.04661600
O	1.88886400	0.01342600	2.07833700
C	4.65769500	2.30123600	1.59043100
C	3.51299600	1.49262300	-0.40227400
C	4.99398300	3.47112900	0.90613400
H	4.97037700	2.13461600	2.62213700
C	3.86671600	2.66095800	-1.06832800
H	2.93074500	0.72845900	-0.91528400
C	4.60021500	3.67387500	-0.42621600
H	5.57894200	4.23956100	1.41726700
H	3.55165400	2.79038700	-2.10667800
C	4.93424200	4.94772900	-1.15472400
H	4.01934200	5.53325200	-1.34755500
H	5.62487200	5.57915300	-0.57847800
H	5.39332400	4.73797000	-2.13353100
C	4.92651600	-1.62423700	0.31635600
C	5.73938900	-2.51698400	1.26359100
C	4.86348700	-2.17330200	-1.08924500
H	5.41401600	-0.63437800	0.26875500
C	7.03190400	-2.97374000	0.58591000
H	5.14374300	-3.40692700	1.53271500
H	5.93341900	-1.97061000	2.19721700
C	5.66559200	-3.15434400	-1.52219700
C	6.73405900	-3.79275200	-0.67473700
H	7.64664100	-3.55677200	1.28858100
H	7.62793100	-2.08644300	0.30917800
H	7.64943900	-3.92496500	-1.27582200
H	6.41689800	-4.81789400	-0.40203000
H	4.12657600	-1.71504100	-1.75512100
H	5.55963900	-3.50884400	-2.55308800

TS1$_a$: (imaginary frequency: 395i cm^{-1})

P	-2.81980600	0.16066700	0.01816500
C	-3.73840400	-0.07752600	-1.55320400
C	-4.87641200	0.68543000	-1.86029500
H	-5.21808300	1.45867900	-1.17103100
C	-5.57412900	0.45855700	-3.04945700

H	-6.45758700	1.05865300	-3.28055700
C	-5.14376800	-0.53007900	-3.93794500
H	-5.68922700	-0.70446900	-4.86869700
C	-4.01339300	-1.29431700	-3.63252900
H	-3.67411100	-2.07040800	-4.32288200
C	-3.30860100	-1.07144400	-2.44834300
H	-2.43236800	-1.67540500	-2.20337100
C	-3.41630700	1.77402600	0.63910000
C	-3.12248700	2.93011500	-0.10403600
H	-2.54153200	2.85240500	-1.02349900
C	-3.56192600	4.17658400	0.33835400
H	-3.32981400	5.07016300	-0.24569400
C	-4.28152400	4.28568900	1.53325600
H	-4.61805000	5.26512300	1.88186000
C	-4.56392700	3.14154900	2.28171900
H	-5.12307500	3.22069600	3.21701900
C	-4.13489800	1.88735000	1.83695400
H	-4.36347200	0.99759500	2.42480100
Pt	-0.51201800	-0.10700000	-0.14316600
Cl	-0.01431000	2.16503700	0.20883300
Cl	-0.78493300	-2.45260400	-0.46235700
C	1.51879000	-0.58200400	-0.05458300
C	2.08198400	-0.90447300	1.28735900
C	1.99568500	-0.66552600	-1.25317500
N	3.51835400	-1.15773100	1.25933700
H	1.54587100	-1.78520400	1.67911800
H	1.87705000	-0.09190800	1.99593000
S	4.54515100	0.01513700	1.91355000
C	4.62957900	1.32065200	0.69457900
O	5.86790200	-0.61175000	1.98389200
O	3.86088500	0.52829100	3.09737500
C	5.80634900	1.49598400	-0.03722900
C	3.49091300	2.08668400	0.42849700
C	5.83113600	2.44497600	-1.06067600
H	6.67990300	0.88639200	0.19784300
C	3.52931000	3.01519900	-0.60805100
H	2.56370300	1.95957700	0.98729300
C	4.69524400	3.21254400	-1.36672600
H	6.74966700	2.58999300	-1.63555600
H	2.61953300	3.57696100	-0.83219300
C	4.72692900	4.24335200	-2.46477300
H	3.78802700	4.24453900	-3.03960200
H	4.84848700	5.25643700	-2.04426800
H	5.56139300	4.07145400	-3.16040900
C	4.01299900	-1.97723000	0.15979500
C	3.37078700	-3.37278600	0.22254500
C	3.84424000	-1.31415000	-1.21291400
H	5.09705500	-2.07825600	0.32179100
C	3.68783200	-4.20442400	-1.01847500
H	2.27682600	-3.27543800	0.29961300
H	3.72041000	-3.86751300	1.14050900
C	3.59624400	-2.07797400	-2.33005100
C	3.16097800	-3.50090200	-2.27435300
H	3.23729600	-5.20452700	-0.93115800
H	4.77774600	-4.35179000	-1.11281800
H	3.46161600	-4.01805400	-3.19986000
H	2.05043400	-3.50653000	-2.26995800
H	4.32761400	-0.34216600	-1.34668900
H	3.64078200	-1.59060600	-3.31074700
H	1.68583100	-0.44060800	-2.26272000
C	-3.53730900	-1.05973300	1.17553200
C	-4.82210900	-1.58705900	0.99059800
C	-2.78679200	-1.43378100	2.30034000
C	-5.35323700	-2.47761400	1.92707000
H	-5.40674200	-1.30611600	0.11268000
C	-3.32410000	-2.31624700	3.23772200
H	-1.77767700	-1.03598100	2.42714500
C	-4.60722000	-2.84075600	3.05163200
H	-6.35337200	-2.89062200	1.77538900
H	-2.73472800	-2.60418000	4.11133300
H	-5.02373000	-3.53864500	3.78206200

TS1$_b$: (imaginary frequency: 400i cm^{-1})

C	3.72557500	-0.17595100	1.61738700
C	4.83232200	0.61201900	1.96080500
H	5.13685400	1.44102500	1.31946000
C	5.54840400	0.33546800	3.12953100
H	6.41095200	0.95200400	3.39436900
C	5.16207000	-0.72386900	3.95459300
H	5.72238900	-0.93746600	4.86821000
C	4.05650800	-1.50843500	3.61048900
H	3.75183100	-2.33751100	4.25394800
C	3.33371200	-1.23781300	2.44639400
H	2.47147100	-1.85101200	2.17258700
C	3.45102300	1.85011600	-0.62152100
C	3.06338400	3.02485000	0.03990200
H	2.33125300	2.98234600	0.84711800
C	3.59631800	4.25262400	-0.35572000
H	3.29063500	5.16604900	0.15997500
C	4.50586500	4.31632600	-1.41637800
H	4.91653300	5.28007000	-1.72730300
C	4.88291200	3.14790300	-2.08260100
H	5.58894000	3.19346500	-2.91533400
C	4.35766600	1.91384100	-1.68681300
H	4.65681700	1.00350500	-2.20917400
Pt	0.30493700	-0.10541300	0.14255200
Cl	-0.15058900	2.17143600	-0.24294800
Cl	0.61012000	-2.43955600	0.49524700
C	-1.70678000	-0.57578600	0.04976500
C	-2.27776400	-0.89945400	-1.28947100
C	-2.17728300	-0.65193900	1.25197500
N	-3.71493600	-1.14410100	-1.25706000
H	-1.74771200	-1.78420700	-1.68046200
H	-2.06965200	-0.09058300	-2.00126600
S	-4.73566400	0.03493300	-1.91062700
C	-4.80270300	1.34588300	-0.69660500
O	-6.06347300	-0.58205500	-1.97156200
O	-4.05303900	0.53806200	-3.09961100
C	-5.97197000	1.53023000	0.04494000
C	-3.65815200	2.10790700	-0.44435200
C	-5.98299600	2.48389800	1.06432400
H	-6.85068700	0.92412300	-0.17967400
C	-3.68275800	3.04118700	0.58826000
H	-2.73698100	1.97433800	-1.01150400
C	-4.84079500	3.24741500	1.35664000
H	-6.89565200	2.63598400	1.64667900
H	-2.76848100	3.59989300	0.80139600
C	-4.85696800	4.28303200	2.45043800
H	-5.69148600	4.12435700	3.14910800
H	-3.91650700	4.27488000	3.02272400
H	-4.96685100	5.29579200	2.02604300
C	-4.21355900	-1.96249200	-0.15786200
C	-3.57435700	-3.35968300	-0.21787000
C	-4.04588000	-1.29886800	1.21344600
H	-5.29749000	-2.06119600	-0.32247200
C	-3.89205600	-4.18700400	1.02597100
H	-2.48022200	-3.26517700	-0.29588500
H	-3.92548000	-3.85628400	-1.13422100
C	-3.78792800	-2.05687900	2.33101000
C	-3.36005100	-3.48262100	2.27911400
H	-3.44576500	-5.18911200	0.94008500
H	-4.98237700	-4.32978200	1.12264200
H	-3.66404700	-3.99485800	3.20631500
H	-2.24976000	-3.49500400	2.27560700

H	-4.51948100	-0.32190400	1.34480100
H	-3.82433700	-1.56535700	3.30994200
H	-1.87011600	-0.42802900	2.26229200
C	3.47695100	-1.11921500	-1.26929400
C	4.76922800	-1.63094500	-1.10305500
C	2.70390700	-1.50550100	-2.37156100
C	5.28996700	-2.52219300	-2.04542000
H	5.36749900	-1.33916500	-0.23713000
C	3.23003600	-2.39212500	-3.31307000
H	1.68767300	-1.11989100	-2.48098400
C	4.52241800	-2.90103500	-3.15068700
H	6.29748100	-2.92416500	-1.91347700
H	2.62547400	-2.69359900	-4.17171800
H	4.93039000	-3.59978600	-3.88512500
As	2.72028700	0.15493600	-0.01767000

TS1$_c$: (imaginary frequency: 156i cm^{-1})

C	2.60905300	-2.54768000	-1.29148900
C	3.55607700	-3.46742400	-0.82332300
H	3.77683700	-3.54731400	0.24249800
C	4.21758800	-4.29557200	-1.73236500
H	4.95788500	-5.01356200	-1.37270900
C	3.92646500	-4.21191200	-3.09823600
H	4.44387400	-4.86412500	-3.80537000
C	2.96437000	-3.30800600	-3.55791500
H	2.72362600	-3.25646100	-4.62193600
C	2.29875100	-2.47584300	-2.65489300
H	1.53390800	-1.77893400	-3.00350900
C	1.47150800	-2.27749200	1.58389600
C	0.20489600	-2.75866800	1.94102800
H	-0.63499800	-2.63749200	1.25611200
C	0.03167500	-3.40005100	3.17057800
H	-0.95780900	-3.76816300	3.45047500
C	1.11469700	-3.56838500	4.03764700
H	0.97403100	-4.06965100	4.99781300
C	2.37951200	-3.09317800	3.67703000
H	3.22752900	-3.22208400	4.35334800
C	2.55993000	-2.44367300	2.45409600
H	3.54509500	-2.05142300	2.19126900
Pt	-0.26057700	-0.14806000	-0.88460000
Cl	-1.18718000	-2.28965800	-1.25209900
Cl	0.74845200	1.99960800	-0.72097100
C	-2.09088000	0.85037100	-1.10001600
C	-2.40675100	1.87597500	-0.04673800
C	-2.74507100	0.38629700	-2.10419200
N	-3.81671100	2.00708600	0.25303200
H	-1.98365000	2.83576600	-0.38353000
H	-1.88405200	1.64011700	0.88331300
S	-4.39011100	1.35967200	1.70938100
C	-4.77314000	-0.34800500	1.36361100
O	-5.64639300	2.05220700	1.98833000
O	-3.25188800	1.40014200	2.63024900
C	-6.10997200	-0.74155600	1.27786900
C	-3.73350800	-1.24931100	1.11167700
C	-6.40479500	-2.05924000	0.92374900
H	-6.89869800	-0.01801400	1.48820200
C	-4.04768600	-2.55562200	0.74895400
H	-2.69222300	-0.93315400	1.17980700
C	-5.38397600	-2.98326800	0.65005100
H	-7.44893100	-2.37483000	0.85732200
H	-3.23734600	-3.24754500	0.51342800
C	-5.70173300	-4.40797800	0.28165200
H	-5.02832400	-4.77717200	-0.50686700
H	-5.57353000	-5.07161600	1.15387900
H	-6.73897200	-4.51675600	-0.06596500
C	-4.75435200	2.16661200	-0.85566800
C	-4.45799300	3.46167300	-1.62624600
C	-4.79385800	0.94370100	-1.76326200
H	-5.75320500	2.25741000	-0.39888200
C	-5.24023500	3.52680400	-2.93662800
H	-3.38128000	3.51710100	-1.85394100
H	-4.69093400	4.31371100	-0.97162800
C	-4.87073800	1.05333900	-3.12270500
C	-4.86073500	2.35824200	-3.85323100
H	-5.05545400	4.48374300	-3.44667500
H	-6.32291900	3.48533600	-2.72715500
H	-5.54258300	2.28290400	-4.71657600
H	-3.85606000	2.51142300	-4.29205000
H	-4.98992800	-0.02048000	-1.28759200
H	-4.97473600	0.13728000	-3.71448400
H	-2.76077500	-0.39416600	-2.84985700
As	1.69106300	-1.33537300	-0.09822900
C	2.98728200	-0.02687200	0.45783000
C	3.03644100	1.06002000	1.31494300
C	3.82144200	1.02584100	0.13938300
N	2.52720900	1.62350000	2.38247200
N	4.64191800	1.57503200	-0.72479800
C	2.98875800	2.93640200	2.89545800
C	1.35488100	0.96914400	3.03844800
C	5.21864900	2.91898500	-0.48879200
C	4.89060700	0.89850100	-2.02943300
H	2.41590800	3.08521000	3.82012700
C	2.62357900	4.07427100	1.94195400
C	4.46546700	2.88137400	3.28517200
H	1.15223600	0.07955100	2.43228200
C	0.11936000	1.86402200	2.97690400
C	1.70577500	0.50825700	4.44983200
H	4.89527800	3.19005700	0.52225700
C	4.63393500	3.94414900	-1.46022400
C	6.74565500	2.87691700	-0.49064900
H	5.61348100	1.54615200	-2.54289400
C	3.61786300	0.84908500	-2.87389900
C	5.54892500	-0.46294700	-1.82212200
H	3.12088200	3.97181800	0.96891800
H	2.92183400	5.03962900	2.37760000
H	1.54243600	4.09425100	1.75299100
H	4.63938800	2.09833400	4.03788900
H	4.78168200	3.84500400	3.71113900
H	5.11522200	2.66869400	2.42311400
H	0.20659400	2.73943300	3.63866300
H	-0.77128400	1.30213700	3.29256800
H	-0.04248200	2.20963600	1.94772100
H	2.58773900	-0.14795800	4.44452800
H	0.86227800	-0.06021700	4.86814400
H	1.89998600	1.35776500	5.12330500
H	4.97803500	4.95312900	-1.18787400
H	3.53425700	3.92849300	-1.42838800
H	4.95336800	3.75457600	-2.49633200
H	7.15295800	2.62591700	-1.48183600
H	7.12127300	2.13945000	0.23466400
H	7.14294600	3.86493200	-0.21426200
H	3.83466200	0.37972600	-3.84461500
H	3.21683300	1.85613000	-3.04918100
H	2.82523100	0.26618600	-2.38927600
H	4.88634200	-1.16091100	-1.29438500
H	6.48288800	-0.36341000	-1.24936100
H	5.78673600	-0.91541500	-2.79582400

Int$_a$:

C	3.92660600	-0.92682300	-0.55367100
C	5.27441000	-0.92304000	-0.16014400
H	5.64997300	-0.13437500	0.49350000
C	6.13793500	-1.92955600	-0.59937900
H	7.18466100	-1.91897600	-0.28595500

C	5.66478100	-2.94543700	-1.43420200
H	6.34090100	-3.73359900	-1.77451300
C	4.32446700	-2.95070200	-1.83104200
H	3.94949700	-3.74156800	-2.48511100
C	3.45526700	-1.94922300	-1.39400000
H	2.41290700	-1.94579700	-1.71657500
C	3.58833900	1.15654000	1.41615000
C	3.81093700	0.36672000	2.55756800
H	3.49533200	-0.67653300	2.56799400
C	4.42512900	0.91779300	3.68127100
H	4.59396500	0.29571900	4.56330500
C	4.80994400	2.26265700	3.68594400
H	5.28550300	2.69309300	4.57059600
C	4.58254300	3.05355600	2.55811900
H	4.88090300	4.10466900	2.55450000
C	3.97589500	2.50387400	1.42477300
H	3.80944100	3.12702700	0.54532900
Pt	0.47762700	-0.41274500	0.24789600
Cl	0.66736900	-0.43364100	2.58246300
Cl	0.32928600	-0.45985000	-2.13707800
C	-1.31596800	-1.15554800	0.34061800
C	-2.41427800	-0.57606700	-0.47991100
C	-1.59076100	-2.36356500	1.08051500
N	-3.75539600	-1.09934300	-0.23759200
H	-2.11456200	-0.74337400	-1.53495100
H	-2.40422200	0.52041600	-0.39179500
S	-4.52436700	-0.35363600	1.09518200
C	-4.87134300	1.25768800	0.41603100
O	-3.58206300	-0.17719100	2.20833700
O	-5.77916200	-1.08466700	1.29201400
C	-4.20171000	2.36906300	0.92413400
C	-5.82483000	1.37934400	-0.59962900
C	-4.48910000	3.62900600	0.39234500
H	-3.47142400	2.23742100	1.72413100
C	-6.09628500	2.64144300	-1.11648800
H	-6.33954000	0.49170200	-0.97022000
C	-5.43392100	3.78541300	-0.63099100
H	-3.96834300	4.50661000	0.78307900
H	-6.83892400	2.74847800	-1.91161700
C	-5.74675400	5.14222900	-1.20535500
H	-5.55866600	5.16520400	-2.29128700
H	-6.80896100	5.39772800	-1.05735600
H	-5.13982500	5.93029300	-0.73766500
C	-3.82597700	-2.57573200	-0.21746200
C	-3.64753200	-3.09860800	-1.67258200
C	-2.85878800	-3.15119700	0.82701900
H	-4.83972200	-2.81819800	0.11889400
C	-2.66155600	-4.25885700	-1.81275400
H	-3.29781000	-2.26919200	-2.30529500
H	-4.63483400	-3.37822200	-2.06935700
C	-1.56264100	-3.73271700	0.35489400
C	-1.32934700	-3.91434500	-1.13885700
H	-2.51045700	-4.48334800	-2.88071900
H	-3.07614000	-5.17301600	-1.35229500
H	-0.59733900	-4.72133100	-1.28941900
H	-0.88775100	-3.01718200	-1.60188700
H	-3.33125300	-3.58676900	1.71126400
H	-1.12205300	-4.50413000	0.99180400
H	-1.10491700	-2.38264700	2.06147800
C	2.89426700	1.67844500	-1.33092000
C	4.01042600	1.78443600	-2.17048800
C	1.84571700	2.60337500	-1.44979500
C	4.07967000	2.81082900	-3.11605200
H	4.82465900	1.06219200	-2.08937700
C	1.92231000	3.63274800	-2.38839600
H	0.96607400	2.50340300	-0.80993700
C	3.03887500	3.73703700	-3.22415400
H	4.95024700	2.88534900	-3.77210900
H	1.10215400	4.34913400	-2.47637600
H	3.09435800	4.53806700	-3.96531700
P	2.76634400	0.39593100	-0.03236100

Int_b:

As	-2.55505800	0.03869100	0.06914200
C	-3.51452900	-1.06706900	-1.21484800
C	-4.70335400	-0.62881100	-1.81386600
H	-5.10473700	0.35862700	-1.57871700
C	-5.37591000	-1.45723000	-2.71710500
H	-6.30242800	-1.11175600	-3.18224600
C	-4.86511700	-2.72123200	-3.02404200
H	-5.39159100	-3.36665500	-3.73140700
C	-3.67942500	-3.15823700	-2.42539000
H	-3.27794200	-4.14662000	-2.66189400
C	-3.00050300	-2.33562600	-1.52343800
H	-2.07990700	-2.68040000	-1.04765900
C	-3.39365900	1.77619200	-0.18071500
C	-3.16849900	2.47184600	-1.37856800
H	-2.51482500	2.04920400	-2.14232400
C	-3.76804600	3.71529900	-1.58441100
H	-3.59154600	4.25223700	-2.51954800
C	-4.58311300	4.27677700	-0.59589600
H	-5.04785300	5.25222900	-0.75901600
C	-4.79922100	3.58989000	0.60084800
H	-5.43329900	4.02464100	1.37732700
C	-4.20735300	2.34009800	0.80988600
H	-4.38433800	1.80574700	1.74479000
Pt	-0.02544500	-0.20184000	-0.05833100
Cl	0.13057500	1.86526100	-1.17895100
Cl	-0.34525800	-2.33930200	0.92354500
C	1.88227500	-0.53696200	-0.16700900
C	2.61432400	-1.19477600	0.95331700
C	2.59932000	-0.30842400	-1.39761700
N	4.06364700	-1.23051600	0.83587800
H	2.19323800	-2.22190100	1.01105700
H	2.32841600	-0.76636700	1.92364200
S	4.88404800	0.02609500	1.62512800
C	4.34837800	1.51524100	0.80322200
O	6.30550700	-0.18197500	1.34422600
O	4.34944400	0.05171500	2.98630200
C	5.04942700	1.97852000	-0.31047300
C	3.15574300	2.12310900	1.21105700
C	4.52064900	3.03884900	-1.04763400
H	5.99311700	1.50754600	-0.58901700
C	2.64437000	3.17903300	0.46371900
H	2.64009800	1.76545300	2.10254700
C	3.30461500	3.63980300	-0.68668500
H	5.05918000	3.40375000	-1.92614500
H	1.69774700	3.63436700	0.75770800
C	2.68171700	4.72216200	-1.52396200
H	1.75382200	4.34250200	-1.98375000
H	2.40486900	5.59461200	-0.91114800
H	3.35408000	5.06083700	-2.32524100
C	4.58221400	-1.70278300	-0.45567200
C	4.39189100	-3.25071200	-0.53120900
C	3.97206800	-0.91010300	-1.62176500
H	5.65553500	-1.48907900	-0.43693400
C	3.68124200	-3.75793200	-1.78804100
H	3.81407300	-3.56303500	0.35164400
H	5.37520400	-3.73227900	-0.42499800
C	2.81810100	-1.50801200	-2.36032600
C	2.41310400	-2.94355900	-2.06242700
H	3.43986900	-4.82572700	-1.66516600
H	4.34995800	-3.68508200	-2.66382100
H	1.86823100	-3.34801600	-2.92777800

H	1.71575400	-3.01388400	-1.21235000
H	4.66798900	-0.28880900	-2.18996800
H	2.69920700	-1.19775700	-3.40171500
H	2.29932600	0.60630500	-1.91835400
C	-3.27944200	-0.53434900	1.77626400
C	-4.53622900	-1.14232500	1.87863400
C	-2.51642300	-0.30306200	2.92829600
C	-5.03096600	-1.50929400	3.13320600
H	-5.12769200	-1.33528100	0.98097200
C	-3.01663200	-0.66611300	4.18046100
H	-1.52522400	0.14857500	2.84254900
C	-4.27381800	-1.26953400	4.28358300
H	-6.01042300	-1.98741900	3.21138000
H	-2.41824800	-0.48714900	5.07680900
H	-4.66152100	-1.55987500	5.26304000

Int$_c$:

As	2.00775800	-1.33049600	-0.33583700
N	3.95135600	2.20296400	0.34707400
N	1.33937900	1.17967200	2.84014100
C	2.60596500	0.06461000	0.86007000
C	3.13477700	1.34183700	0.90624200
C	2.15295600	0.93037500	1.84020300
C	4.13512800	3.58626200	0.84849700
H	4.93898500	3.99881000	0.22474200
C	4.64358700	3.58951500	2.29013500
H	3.93516100	3.11557700	2.98478500
H	4.80649900	4.62202000	2.63272200
H	5.59797100	3.04781600	2.36363800
C	2.88902400	4.43686000	0.59990400
H	2.63238300	4.44496000	-0.46818400
H	3.06775000	5.47296600	0.92418600
H	2.01300600	4.05672400	1.14057700
C	4.71452000	1.77044900	-0.85721500
H	4.38887500	0.74309400	-1.04300100
C	6.21436800	1.73894200	-0.57017600
H	6.62912200	2.74438600	-0.39716500
H	6.73996600	1.30848000	-1.43528000
H	6.43681300	1.11378400	0.30777300
C	4.34652600	2.60262500	-2.08249200
H	3.26426000	2.55875700	-2.26718800
H	4.86292000	2.19343100	-2.96288200
H	4.65247800	3.65527100	-1.97696700
C	1.14445500	2.57656700	3.31081800
H	1.98311200	3.13532900	2.88224900
C	1.24340900	2.70502600	4.82839100
H	1.20094400	3.76983600	5.10116300
H	2.19268900	2.29511600	5.20441500
H	0.41455000	2.20385500	5.34906000
C	-0.15091400	3.14184600	2.72673000
H	-1.04044000	2.58294000	3.05250200
H	-0.11520200	3.10402000	1.62706500
H	-0.27458000	4.19171000	3.03274000
C	0.51488600	0.09946400	3.46041200
H	-0.21318700	0.63775700	4.07921300
C	1.38801600	-0.77578900	4.35908500
H	0.76476900	-1.52240200	4.87339700
H	1.91278400	-0.18221500	5.12099900
H	2.13316600	-1.32244400	3.76116500
C	-0.27415700	-0.72152200	2.45037400
H	0.35652500	-1.44021100	1.91283900
H	-0.78927400	-0.07682400	1.73050200
H	-1.04028300	-1.30388100	2.98111700
C	3.39766600	-1.35602400	-1.68746800
C	4.64629100	-1.94945400	-1.45698200
H	4.85191000	-2.45678900	-0.51236200
C	5.63084700	-1.88881200	-2.44531300
H	6.60605100	-2.34821400	-2.26914100
C	5.36582900	-1.24919500	-3.66182100
H	6.13744400	-1.20779200	-4.43392500
C	4.11268700	-0.67569500	-3.89597800
H	3.90266000	-0.18569000	-4.84918900
C	3.12319600	-0.72821200	-2.91062700
H	2.14982400	-0.26365500	-3.08264500
C	2.33876500	-2.90571000	0.74074500
C	1.61244600	-4.07479900	0.47549500
H	0.83900800	-4.07696200	-0.29371600
C	1.86459400	-5.22650800	1.22603700
H	1.29656900	-6.13689000	1.02256100
C	2.83192300	-5.21481100	2.23448200
H	3.02255900	-6.11735700	2.81936400
C	3.55537500	-4.04734400	2.49784600
H	4.31133900	-4.03572500	3.28624600
C	3.31150700	-2.89177700	1.75254200
H	3.87806500	-1.98143900	1.96178500
Pt	-0.29349700	-0.40773200	-1.01909800
Cl	-1.22756800	-2.56171700	-0.89698100
Cl	0.76124900	1.71722000	-1.29146200
C	-2.02976600	0.42713500	-1.21639800
C	-2.27074400	1.68495500	-0.44029300
C	-3.10509500	-0.09664200	-1.99164000
N	-3.65126900	1.90610300	-0.06064100
H	-1.89813900	2.52231300	-1.06552100
H	-1.64482000	1.72183500	0.45640100
S	-4.15636100	1.36356600	1.46428500
C	-4.78238900	-0.28688500	1.21901800
O	-5.27922800	2.21357600	1.84557400
O	-2.92964500	1.28842100	2.27183100
C	-6.16413800	-0.48805600	1.16796500
C	-3.88974100	-1.34193700	1.01539200
C	-6.64999300	-1.76644700	0.89309600
H	-6.83924200	0.34905300	1.35092800
C	-4.39310000	-2.60992100	0.73783800
H	-2.81322400	-1.18437700	1.05559700
C	-5.77722600	-2.84502000	0.67205400
H	-7.72961200	-1.93096200	0.85300200
H	-3.68954100	-3.42474300	0.55685000
C	-6.30732700	-4.22771200	0.40210900
H	-5.65112500	-4.78287300	-0.28462600
H	-6.36453900	-4.80868800	1.33870400
H	-7.31906900	-4.19864800	-0.02759400
C	-4.63125400	1.87939500	-1.15068500
C	-4.55415400	3.22084600	-1.94761100
C	-4.46932400	0.60814000	-2.00570100
H	-5.61732300	1.82398100	-0.67591200
C	-4.27863900	3.07775100	-3.44628700
H	-3.75952600	3.82839100	-1.48906300
H	-5.48502600	3.78236400	-1.78314100
C	-3.65612200	0.70134900	-3.23785300
C	-3.16065500	2.06007000	-3.70049700
H	-4.01334500	4.06002600	-3.86668500
H	-5.18766400	2.74647400	-3.97688300
H	-2.90734400	2.00531400	-4.76856500
H	-2.23820500	2.37011700	-3.18599200
H	-5.31506000	-0.08442900	-1.99725100
H	-3.89440400	-0.00440200	-4.03793100
H	-3.06340000	-1.17163300	-2.17814800

TS2$_a$: (imaginary frequency: 1025i cm^{-1})

P	-2.87154200	0.34956500	0.04946300
C	-3.69568000	0.53039300	-1.58200100
C	-4.64934100	1.53226800	-1.82118500
H	-4.89924700	2.24715400	-1.03612200
C	-5.28054400	1.62044000	-3.06476000

H	-6.01985000	2.40549400	-3.24146900
C	-4.96751900	0.70939500	-4.07668100
H	-5.46047500	0.78054900	-5.04942300
C	-4.02209100	-0.29316700	-3.84015300
H	-3.77578600	-1.01068400	-4.62662300
C	-3.38478900	-0.38532300	-2.60139500
H	-2.65725400	-1.17722000	-2.41188500
C	-3.20091300	1.94578100	0.88437400
C	-2.64227400	3.11519400	0.34077600
H	-2.02457800	3.05609600	-0.55585100
C	-2.86691000	4.34835400	0.95066200
H	-2.42928000	5.25204700	0.51999800
C	-3.63570100	4.42723600	2.11681200
H	-3.80479500	5.39421400	2.59690500
C	-4.18270300	3.26684800	2.66759900
H	-4.78253000	3.32113200	3.57925500
C	-3.96915200	2.02890200	2.05351000
H	-4.40462700	1.12765300	2.48685700
Pt	-0.62108000	-0.36057900	-0.09355300
Cl	0.26818000	1.72924200	0.57192000
Cl	-1.35621900	-2.53648900	-0.70060000
C	1.28880100	-1.02938900	-0.31890400
C	2.26973800	-0.81210600	0.66282200
C	1.73330900	-1.64637000	-1.58631000
N	3.61201700	-1.10040600	0.50040900
H	1.47072400	-1.83714700	0.81133400
H	2.02781100	-0.20456200	1.53903700
S	4.72576200	-0.24138700	1.47918400
C	5.02355500	1.22266400	0.50742200
O	5.95120700	-1.03740100	1.51436600
O	3.99727000	0.11788700	2.69178000
C	6.30313700	1.45448500	0.00477300
C	3.96592700	2.10803200	0.26278900
C	6.52665000	2.59986300	-0.76311300
H	7.10443000	0.74569300	0.21762100
C	4.21086500	3.23617300	-0.51290800
H	2.95872800	1.92721700	0.64711200
C	5.49021300	3.50414600	-1.03479000
H	7.52683600	2.79176300	-1.15936300
H	3.38481400	3.92193500	-0.71765300
C	5.72903200	4.74226300	-1.85802700
H	5.00665300	4.81305300	-2.68699600
H	5.60381200	5.65014400	-1.24461700
H	6.74269100	4.75888000	-2.28296200
C	4.13318900	-1.96777700	-0.58476100
C	4.39497100	-3.37391400	-0.02728800
C	3.19291600	-2.01063200	-1.78821000
H	5.08324200	-1.52271000	-0.90878800
C	3.08967900	-4.03483300	0.41380200
H	5.10274700	-3.29737300	0.80946100
H	4.87902500	-3.97053600	-0.82031900
C	2.13540100	-3.08921000	-1.80250100
C	2.08409000	-4.18342500	-0.74612100
H	2.66055500	-3.45195200	1.24612600
H	3.29602500	-5.02780100	0.84169300
H	2.30484900	-5.12832700	-1.26892600
H	1.05117200	-4.26959600	-0.37154900
H	3.65139300	-1.71666200	-2.73538800
H	1.84217300	-3.44178900	-2.79461700
H	1.19765300	-1.21297300	-2.43331600
C	-3.91257800	-0.84735200	0.96217100
C	-5.26161800	-1.05183100	0.64370300
C	-3.34017800	-1.54161500	2.03851200
C	-6.03261600	-1.93798900	1.40018900
H	-5.70936500	-0.52186800	-0.19894100
C	-4.11528700	-2.41931600	2.79727800
H	-2.28260000	-1.39617900	2.26836200
C	-5.46208500	-2.61983000	2.47855000
H	-7.08267800	-2.09780200	1.14376900
H	-3.66323600	-2.95793600	3.63339700
H	-6.06610800	-3.31406900	3.06788700

$TS2_b$: (imaginary frequency: 878i cm^{-1})

C	-4.07284200	-0.98062100	-0.77117600
C	-5.29851900	-0.60037200	-1.33367600
H	-5.60090100	0.44857900	-1.33161400
C	-6.13504200	-1.56579800	-1.90237900
H	-7.08988400	-1.26481900	-2.34058200
C	-5.75088900	-2.90926700	-1.91122300
H	-6.40555300	-3.66238400	-2.35679500
C	-4.52649300	-3.28778200	-1.35137500
H	-4.22244600	-4.33743100	-1.35724700
C	-3.68416200	-2.32871500	-0.78437300
H	-2.72904100	-2.62420600	-0.34409700
C	-3.67321400	2.00255900	-0.49677100
C	-3.48303700	2.42247800	-1.82209700
H	-2.86321900	1.83263000	-2.49831700
C	-4.06586000	3.61090500	-2.26547700
H	-3.91439300	3.93435900	-3.29812500
C	-4.82940600	4.39041100	-1.39051100
H	-5.28116300	5.32212500	-1.73995800
C	-5.00813600	3.97943100	-0.06742400
H	-5.59965200	4.58736100	0.62160900
C	-4.43209200	2.78667600	0.38114400
H	-4.57818800	2.46901900	1.41504800
Pt	-0.48796900	-0.12426000	-0.28237000
Cl	-0.18794300	1.71338200	-1.71991100
Cl	-0.60927300	-2.04575000	1.12826400
C	1.46194800	-0.60701100	-0.55386000
C	2.38837800	-0.63841100	0.49185900
C	1.95782800	-0.95583000	-1.90464800
N	3.71016100	-1.02672300	0.33858200
H	1.47909700	-1.61527200	0.38244700
H	2.13753200	-0.25668100	1.48444300
S	4.83836200	-0.56901800	1.53680600
C	5.60067000	0.86254300	0.79885300
O	5.84076900	-1.62829600	1.61913900
O	4.04845800	-0.14985400	2.69203900
C	6.90302400	0.77190100	0.31029900
C	4.86633600	2.05068700	0.70678700
C	7.47485800	1.89420900	-0.29413400
H	7.45454400	-0.16356500	0.41299600
C	5.45211700	3.15458200	0.09700900
H	3.85289600	2.10788300	1.10804400
C	6.76256200	3.09547900	-0.41463800
H	8.49607000	1.83329500	-0.67802100
H	4.88400200	4.08471700	0.01604000
C	7.37262200	4.30464300	-1.07257900
H	8.39912100	4.10788100	-1.41242600
H	6.77772000	4.61957600	-1.94552700
H	7.40055800	5.15967900	-0.37758600
C	4.20380700	-1.76761200	-0.85181900
C	4.23416100	-3.27487600	-0.55938100
C	3.37325600	-1.45343700	-2.09288500
H	5.22778500	-1.41256500	-1.03100900
C	2.82545100	-3.83177700	-0.36176700
H	4.85736800	-3.45588700	0.32655300
H	4.72353400	-3.76947900	-1.41689100
C	2.19838200	-2.35954500	-2.40387100
C	1.92439300	-3.62325500	-1.59670200
H	2.37403500	-3.37811200	0.53583300
H	2.87818500	-4.90736200	-0.13379900
H	2.07739000	-4.47304900	-2.28155000
H	0.86476800	-3.64968400	-1.29466200

H	3.94013100	-1.03801800	-2.92939500
H	1.97128300	-2.46922900	-3.46785100
H	1.55608100	-0.25137000	-2.63820700
C	-3.39005000	0.20870200	1.93723600
C	-4.65738300	-0.23165700	2.33788500
C	-2.44887800	0.60074600	2.89807400
C	-4.98445600	-0.26897500	3.69611700
H	-5.38804000	-0.55058300	1.59129500
C	-2.78086500	0.56628300	4.25418000
H	-1.45281000	0.91863700	2.58095700
C	-4.04826800	0.13192800	4.65403100
H	-5.97285700	-0.61621600	4.00706700
H	-2.04377700	0.86977900	5.00140600
H	-4.30475800	0.09899200	5.71576600
As	-2.88397200	0.31712700	0.06498100

TS2$_c$: (imaginary frequency: 942i cm^{-1})

As	2.19750000	-1.34918900	-0.34188400
N	3.76138300	2.28042000	-0.58456400
N	3.28229800	1.01324400	2.92144200
C	3.24217800	0.01733500	0.52747900
C	3.57283600	1.34460300	0.31545700
C	3.38354100	0.84833200	1.62370200
C	4.08759700	3.68435600	-0.23590200
H	4.22914100	4.17982400	-1.20563000
C	5.41896400	3.76540200	0.50997800
H	5.39205100	3.21994400	1.46514200
H	5.66866500	4.81366500	0.73089400
H	6.23062100	3.33788000	-0.09685600
C	2.92128100	4.38000300	0.46620400
H	2.00716200	4.31823500	-0.13877200
H	3.16325400	5.44037600	0.63285100
H	2.69462100	3.92663600	1.43952100
C	3.53497700	1.92967700	-2.01578900
H	3.27341600	0.86663900	-2.00904000
C	4.81680600	2.08643500	-2.82951000
H	5.13498200	3.13798000	-2.90725500
H	4.65050500	1.71296800	-3.85056300
H	5.63735100	1.50257400	-2.38767500
C	2.34230600	2.68959800	-2.59276600
H	1.44772900	2.51895700	-1.97813700
H	2.14163200	2.32377000	-3.61084800
H	2.53190800	3.77210100	-2.66212700
C	3.52264500	2.33530000	3.54591700
H	3.87449800	2.97360100	2.72783300
C	4.63660400	2.26479000	4.58912700
H	4.85519400	3.27536800	4.96508600
H	5.55973000	1.85197600	4.15503400
H	4.35568700	1.64683600	5.45551200
C	2.22088400	2.93123100	4.08210100
H	1.83279200	2.36011600	4.93905300
H	1.44848900	2.94762400	3.29913100
H	2.39667100	3.96196900	4.42450700
C	2.78607300	-0.10591400	3.77244800
H	2.82035400	0.29183700	4.79523100
C	3.72854600	-1.30465500	3.70574000
H	3.38660000	-2.08664300	4.39916800
H	4.75165100	-1.01524600	3.98817000
H	3.75346000	-1.75002700	2.70302900
C	1.33140700	-0.44491500	3.44884300
H	1.21185200	-0.80507600	2.41973700
H	0.68131600	0.43233300	3.56495700
H	0.97784900	-1.23901300	4.12271400
C	3.25332100	-1.62333900	-1.94419700
C	4.64776000	-1.46489500	-1.93834400
H	5.16902300	-1.18177100	-1.02076300
C	5.37223700	-1.64675300	-3.11792400
H	6.45742200	-1.52172000	-3.11417800
C	4.70808400	-1.98641900	-4.30124600
H	5.27636900	-2.12748900	-5.22335700
C	3.31970700	-2.14675200	-4.30388600
H	2.80135000	-2.41500900	-5.22709100
C	2.58527500	-1.96625900	-3.12801900
H	1.50069700	-2.09800300	-3.12389100
C	2.45355700	-2.94461300	0.72184200
C	1.36002900	-3.43248300	1.44801400
H	0.39043700	-2.93635800	1.37495300
C	1.51672200	-4.56184600	2.25561900
H	0.66497300	-4.94579300	2.82122400
C	2.75585900	-5.20362500	2.33007000
H	2.87546300	-6.08759700	2.96049700
C	3.84094200	-4.72554200	1.58709800
H	4.80527200	-5.23617100	1.63449200
C	3.69144700	-3.59859700	0.77693600
H	4.53778000	-3.23737900	0.18997700
Pt	-0.08777100	-0.45739900	-0.56828400
Cl	-0.63545900	-2.49987000	-1.60464500
Cl	0.37318700	1.63648700	0.47431700
C	-1.97924900	0.18481400	-0.84289200
C	-2.84874500	0.47342400	0.22736400
C	-2.54398900	0.29132500	-2.20698400
N	-4.15495500	0.88243600	0.03722300
H	-1.95919300	1.39171500	-0.08635900
H	-2.57821800	0.22520200	1.25735700
S	-5.17501000	1.04653100	1.42169100
C	-6.49698600	-0.06786500	1.02441600
O	-5.70075500	2.40906000	1.42978200
O	-4.38718100	0.50884000	2.53106400
C	-7.72558900	0.45077700	0.61490700
C	-6.28409700	-1.44624400	1.14145000
C	-8.75681400	-0.43681800	0.30121800
H	-7.86831900	1.53066700	0.55843900
C	-7.32462700	-2.31160700	0.82336800
H	-5.32103500	-1.82713000	1.48524400
C	-8.57579300	-1.82429300	0.39758000
H	-9.72363900	-0.04127800	-0.01842800
H	-7.17082800	-3.38998700	0.91177300
C	-9.69008800	-2.78174600	0.07185900
H	-10.00568000	-3.33349300	0.97279800
H	-10.56955800	-2.26079900	-0.3310580
H	-9.36442200	-3.53146800	-0.66673700
C	-4.48605700	1.66273100	-1.17996000
C	-4.06134300	3.15275700	-0.97822200
C	-3.88299900	0.96370100	-2.39872900
H	-5.57705600	1.61432800	-1.28732700
C	-3.34862200	3.77836900	-2.17510400
H	-3.38459700	3.20460600	-0.10926000
H	-4.94618600	3.73191400	-0.68488900
C	-2.63960300	1.55032200	-3.03590800
C	-2.15100800	2.91364300	-2.57197600
H	-3.03046900	4.80007700	-1.91397100
H	-4.03677700	3.87008900	-3.03316700
H	-1.57127000	3.38398700	-3.37963800
H	-1.46111700	2.82279400	-1.71432000
H	-4.60471400	0.45923500	-3.04465200
H	-2.54844400	1.36671200	-4.10954400
H	-2.33247500	-0.63209600	-2.75565600

Pro-com$_a$:

P	2.19827200	-0.32661400	0.02787400
C	2.69642300	1.23510500	0.88919700
C	3.88606900	1.91168400	0.54108900
H	4.50030600	1.55191800	-0.29021600
C	4.29188800	3.04448700	1.26335300

H	5.21889700	3.55815800	0.98547100
C	3.52038900	3.51045800	2.33813700
H	3.84284700	4.39144300	2.90425700
C	2.33450000	2.84382000	2.68244500
H	1.72442000	3.20286000	3.51852800
C	1.91792800	1.71537200	1.96322500
H	0.99842900	1.18767200	2.24024000
C	3.24082100	-0.33264600	-1.49245500
C	3.02759400	0.66053100	-2.47299700
H	2.24377700	1.41037500	-2.33040600
C	3.81127100	0.68515200	-3.63262100
H	3.63789300	1.46044500	-4.38666500
C	4.80098800	-0.28921100	-3.83838100
H	5.40666600	-0.27207300	-4.75103300
C	5.00607400	-1.28708900	-2.87651200
H	5.77325000	-2.05343500	-3.03169700
C	4.23171800	-1.30974100	-1.70623300
H	4.40316500	-2.09018700	-0.95878300
Pt	-0.05861500	-0.77186700	-0.31095700
Cl	0.08896800	-0.66669600	-2.66171600
Cl	-0.31288900	-0.84744000	2.03965400
C	-1.99947900	-1.92310300	-0.60597700
C	-2.49581300	-0.63329100	-0.84633900
C	-2.44359000	-2.66172300	0.60843500
N	-3.35791600	0.00371600	0.00486200
H	-2.31561100	-0.14780600	-1.81231700
S	-3.83361900	1.63513800	-0.42667700
C	-2.41752100	2.68578700	-0.11342800
O	-4.88988000	1.98514000	0.54257700
O	-4.06433500	1.62866900	-1.88348000
C	-2.38792600	3.43008900	1.07339900
C	-1.43750400	2.84700400	-1.10664000
C	-1.35834600	4.36106800	1.26018900
H	-3.17767200	3.29897300	1.81840300
C	-0.41682100	3.77742600	-0.89380700
H	-1.47829600	2.26749700	-2.03268800
C	-0.36404900	4.55722600	0.28169400
H	-1.33671600	4.95794200	2.17899800
H	0.34895500	3.91183100	-1.66626200
C	0.72803500	5.58522200	0.46682600
H	1.72512000	5.11366600	0.41224800
H	0.68218000	6.35270800	-0.32752800
H	0.64226000	6.09495800	1.44023800
C	-4.18234700	-0.73380400	1.01803100
C	-5.57174900	-1.05236700	0.41622500
C	-3.47659100	-2.00937300	1.49846800
H	-4.30082200	-0.05098800	1.87166400
C	-5.46726700	-2.06007000	-0.73428200
H	-6.05119800	-0.11666400	0.08655800
H	-6.19676100	-1.46638700	1.23169100
C	-3.80579300	-3.31840500	0.79082100
C	-4.92147700	-3.41680200	-0.24561800
H	-4.82786200	-1.63595900	-1.53053000
H	-6.45940200	-2.20985300	-1.19581200
H	-5.75287800	-3.96748700	0.23461000
H	-4.59780600	-4.03719100	-1.10269600
H	-3.27920100	-2.03172800	2.57484500
H	-3.74546900	-4.20379900	1.43684600
H	-1.63074900	-3.16931800	1.13904300
C	2.91500400	-1.67094900	1.06811600
C	3.98522700	-1.43811200	1.95328300
C	2.39596000	-2.97511200	0.93510300
C	4.53081200	-2.49897400	2.69140800
H	4.38889400	-0.42773100	2.07439400
C	2.95008300	-4.03240100	1.66837400
H	1.54790200	-3.14904700	0.26305800
C	4.01718800	-3.79616000	2.54884600
H	5.35843400	-2.30771900	3.38314100
H	2.53952600	-5.04200100	1.55932700
H	4.44359700	-4.62204000	3.12872800
H	-1.64470900	-2.47918900	-1.48227600

Pro-com$_b$:

C	-3.71670800	-1.05974500	-0.73518400
C	-4.78853300	-0.43284200	-1.39938900
H	-4.79198700	0.65274100	-1.54349900
C	-5.85647200	-1.20375600	-1.88503900
H	-6.68800400	-0.71217600	-2.40210000
C	-5.85782200	-2.59533900	-1.71078100
H	-6.69151800	-3.19450000	-2.09323700
C	-4.78909100	-3.21871300	-1.04831200
H	-4.78627900	-4.30548800	-0.91056100
C	-3.71651600	-2.45812400	-0.56107000
H	-2.88364700	-2.94163300	-0.03695200
C	-2.44672000	1.72566500	-0.85772400
C	-2.29017600	1.85323300	-2.25327400
H	-2.02973900	0.98170000	-2.86050800
C	-2.44989900	3.10532300	-2.86331100
H	-2.33022500	3.19680300	-3.94840400
C	-2.75117300	4.23753000	-2.08965900
H	-2.87372300	5.21434900	-2.57065900
C	-2.89613800	4.11490700	-0.70019900
H	-3.13313000	4.99364500	-0.09015500
C	-2.74578600	2.86213700	-0.08303700
H	-2.86676900	2.77335200	1.00161300
Pt	-0.05011500	-1.14079500	-0.21224200
Cl	0.62464800	0.27682900	-1.96634200
Cl	-0.76736300	-2.64198600	1.47428300
C	1.76266900	-2.42456700	-0.39597600
C	2.13725800	-1.53005200	0.63362300
C	2.44945500	-2.35422300	-1.71814900
N	3.14287900	-0.61070500	0.46745100
H	1.76444700	-1.65272700	1.65594400
S	3.30600600	0.66746000	1.65062900
C	2.99334300	2.16713700	0.72568600
O	4.71929600	0.69616400	2.07276400
O	2.21225400	0.43822900	2.61218300
C	4.07533600	2.99961900	0.40193600
C	1.67712600	2.50456900	0.37561400
C	3.82461200	4.18756400	-0.29618100
H	5.08680200	2.71973700	0.70989400
C	1.45051400	3.69403900	-0.32102300
H	0.84969000	1.83955200	0.63356100
C	2.51533400	4.55258300	-0.66928400
H	4.66307100	4.84503700	-0.55256600
H	0.42576100	3.95128100	-0.60974500
C	2.24634600	5.83870500	-1.41707600
H	3.18264000	6.33352600	-1.72272400
H	1.64044200	5.65129000	-2.32143700
H	1.67689700	6.54716100	-0.78701800
C	4.17898100	-0.73251300	-0.60628200
C	5.41493500	-1.48223800	-0.05307100
C	3.62020200	-1.41043600	-1.86489900
H	4.46184200	0.29886200	-0.87358000
C	5.09915700	-2.95772200	0.21981400
H	5.76735900	-0.97658700	0.85920900
H	6.21681700	-1.40182100	-0.81320100
C	3.83283900	-2.91045100	-2.02540500
C	4.72737800	-3.70196700	-1.07733500
H	4.28208300	-3.02618100	0.96223500
H	5.97086600	-3.44894600	0.68763600
H	5.66310400	-3.91962800	-1.62744000
H	4.27154400	-4.68351600	-0.84662900
H	3.63470400	-0.77935400	-2.75904600

H	3.91609200	-3.24278800	-3.06816900
H	1.76035300	-2.37995400	-2.56989100
C	-2.70200000	0.30860800	1.84113100
C	-4.05122100	0.37433300	2.23539400
C	-1.67919900	0.51413000	2.78630300
C	-4.37447000	0.65649300	3.57119800
H	-4.85012600	0.19705000	1.50698000
C	-2.01096700	0.80186000	4.11848200
H	-0.62694500	0.43079300	2.49257600
C	-3.35584500	0.87331600	4.51173000
H	-5.42552100	0.70133100	3.87725800
H	-1.21152700	0.95751000	4.85068000
H	-3.61113700	1.09004400	5.55489200
As	-2.20948100	-0.03106400	-0.02078200
H	1.30464500	-3.36959500	-0.07659300

pro-com$_c$:

As	1.22624300	0.92230000	0.92667600
N	4.58029800	-1.02039000	0.05719800
N	3.15040400	0.97121700	-2.78924000
C	2.75525100	0.77205200	-0.23436800
C	3.80401200	-0.10062500	-0.46257400
C	3.24853600	0.65498900	-1.52112200
C	5.59999700	-1.75554700	-0.73075000
H	6.08259900	-2.41901800	-0.00121100
C	6.67553100	-0.80496800	-1.25537000
H	6.26131900	-0.04246700	-1.93166900
H	7.44022300	-1.36606300	-1.81248800
H	7.16987800	-0.28133800	-0.42394300
C	4.95272900	-2.64108600	-1.79550500
H	4.22018300	-3.32290200	-1.34347900
H	5.72256000	-3.23870500	-2.30619100
H	4.42173300	-2.05250600	-2.55435100
C	4.34402300	-1.42056800	1.47417500
H	3.52386000	-0.78100100	1.81750900
C	5.56440700	-1.11418700	2.33821500
H	6.43119400	-1.73669200	2.06651500
H	5.32708000	-1.31658300	3.39288000
H	5.85145300	-0.05591300	2.25414400
C	3.87085800	-2.86965900	1.57003500
H	2.99134400	-3.02946200	0.93074100
H	3.59129200	-3.08900400	2.61136700
H	4.65852100	-3.58400900	1.28400500
C	4.05800200	0.38165600	-3.80140800
H	4.77773600	-0.20958700	-3.22485300
C	4.83727100	1.46499000	-4.54540600
H	5.56312000	0.99641500	-5.22645900
H	5.38911300	2.10816200	-3.84339900
H	4.17957400	2.10300100	-5.15489600
C	3.30069800	-0.56918100	-4.72809200
H	2.58432200	-0.03182200	-5.36783900
H	2.74685100	-1.32267100	-4.14877100
H	4.01125000	-1.08741500	-5.38919500
C	2.02254500	1.83478000	-3.24895800
H	2.19907000	1.96724000	-4.32462300
C	2.09254400	3.21335200	-2.59604000
H	1.28449900	3.84975800	-2.98434500
H	3.05426200	3.70170600	-2.81345100
H	1.96527400	3.16125100	-1.50723300
C	0.68484300	1.12158700	-3.07263600
H	0.48317700	0.87035900	-2.02600200
H	0.65634500	0.18018900	-3.63666100
H	-0.13980900	1.75856600	-3.41990900
C	2.11134400	1.13560400	2.63512200
C	3.34363800	1.80191600	2.72287300
H	3.81750800	2.20962500	1.82683100
C	3.97746800	1.92721400	3.96057700
H	4.93692600	2.44468800	4.02980500
C	3.38514000	1.38789400	5.10727600
H	3.88381700	1.48406400	6.07430600
C	2.15635000	0.72809900	5.01701300
H	1.69228000	0.30989700	5.91288000
C	1.51235900	0.59944600	3.78291400
H	0.54604300	0.09632400	3.71018400
C	0.41875000	2.63036600	0.51727400
C	-0.70988500	2.64338100	-0.31058700
H	-1.13247700	1.71632300	-0.69799500
C	-1.29530100	3.86346000	-0.65489500
H	-2.17644600	3.86932600	-1.29990100
C	-0.76018600	5.06032800	-0.17036800
H	-1.21996000	6.01385900	-0.44008200
C	0.35872700	5.04009600	0.66953100
H	0.76930400	5.97439400	1.05877500
C	0.95025900	3.82445800	1.02081800
H	1.81428400	3.81415900	1.68759200
Pt	-0.19171300	-0.99501800	0.53902200
Cl	-1.59828400	-0.01495500	2.16220800
Cl	1.26750400	-1.98868900	-1.04420000
C	-1.49186400	-2.81141800	0.28862200
C	-1.99272800	-1.96191800	-0.70670400
C	-2.33407900	-3.12265400	1.46969200
N	-3.20885900	-1.36084300	-0.61105000
H	-1.46107300	-1.83894800	-1.65154200
S	-3.56610900	-0.17176200	-1.81982400
C	-4.55355200	1.00296900	-0.93086300
O	-4.37850700	-0.77544000	-2.87401800
O	-2.25797300	0.40332600	-2.15809600
C	-5.81213300	1.32090000	-1.44455100
C	-4.04535600	1.63007100	0.21291200
C	-6.57453900	2.29342800	-0.79578100
H	-6.17919000	0.81184500	-2.33639100
C	-4.82748200	2.58985900	0.84611100
H	-3.07736800	1.34963200	0.62906100
C	-6.09909400	2.94163400	0.35418300
H	-7.55962200	2.55118800	-1.19123200
H	-4.44318600	3.07655100	1.74598800
C	-6.92311300	3.98379900	1.06069400
H	-6.37861600	4.93987100	1.12366200
H	-7.87725700	4.16634800	0.54748800
H	-7.14504000	3.67264500	2.09460200
C	-4.29746300	-1.89006600	0.25728700
C	-5.20043500	-2.83241100	-0.55541200
C	-3.73815400	-2.58099000	1.50024200
H	-4.87334600	-1.01868400	0.59124800
C	-4.43586800	-4.08441500	-0.97750300
H	-5.59933400	-2.30772700	-1.43357400
H	-6.05677200	-3.10295400	0.08587600
C	-3.51185200	-4.07753800	1.43574700
C	-3.96274200	-4.90032900	0.23759800
H	-3.58734400	-3.78928800	-1.61608800
H	-5.07190900	-4.71672900	-1.61515200
H	-4.80868400	-5.51807500	0.58166200
H	-3.17204100	-5.60966100	-0.05872900
H	-4.07397200	-2.14220600	2.44109100
H	-3.64896800	-4.59737500	2.38837100
H	-1.79426500	-3.09862900	2.41924800
H	-0.72056200	-3.52183900	-0.01872600

pro:

C	2.80783200	1.35211000	-1.19552000
C	1.76010100	0.45926800	-1.42259800
C	1.54413200	-0.57965900	-0.51521600
C	2.37398300	-0.75084100	0.59519800
C	3.41801300	0.14775600	0.80374300

C	3.65018100	1.21398900	-0.08128900
H	2.98068600	2.16801600	-1.90206700
H	1.11951300	0.55268300	-2.30055100
H	2.19780300	-1.58038200	1.27963200
H	4.07008600	0.01857500	1.67176500
C	4.79877500	2.16178800	0.14733700
H	4.88963900	2.43338000	1.21051900
H	5.75458800	1.69759800	-0.15080900
H	4.68331900	3.08653900	-0.43630700
S	0.15977200	-1.68587500	-0.76039800
O	-0.18840700	-1.62522000	-2.18151700
O	0.47773100	-2.94833800	-0.08964400
N	-1.13506300	-1.03286600	0.07918900
C	-1.32259300	-1.39562200	1.47949300
H	-1.11103100	-2.46925100	1.58635200
H	-2.39212600	-1.25244000	1.70702200
C	-0.51309100	-0.64546300	2.45061000
C	0.16227100	-0.04703300	3.25785000
H	0.76457700	0.48947600	3.96599600
C	-1.89279800	0.08232800	-0.50816100
C	-3.37439300	-0.20693200	-0.42371200
C	-1.54845100	1.45116600	0.09775000
H	-1.61944600	0.07652400	-1.57545300
C	-4.29603000	0.72659200	-0.15646800
C	-2.53704700	2.51349600	-0.38583000
H	-1.59420200	1.38402600	1.19647000
H	-0.51194700	1.71898500	-0.15658400
C	-3.96410800	2.17899900	0.06470400
H	-2.24209300	3.50912200	-0.01845200
H	-2.50824200	2.56290900	-1.48895500
H	-4.69662200	2.81037600	-0.46705800
H	-4.09302600	2.42258400	1.13708800
H	-3.66635000	-1.24428800	-0.61532600
H	-5.35130600	0.43643000	-0.10929600