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Supporting Information

New Vistas in Transmetalation with Discrete "$AgCF_3$" Species: Implications in Pd-Mediated Trifluoromethylation Reactions

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General Procedures

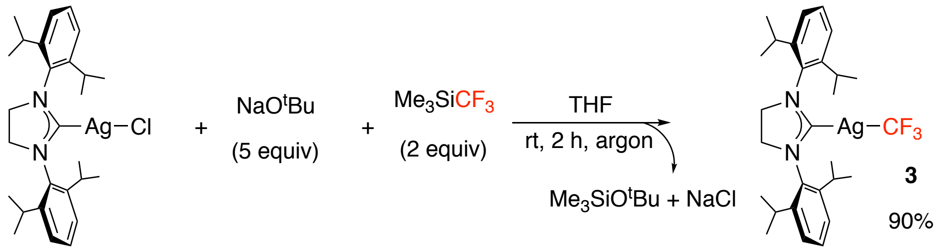
All reactions were conducted in an argon-filled glovebox (mBraun Unilab 4420) with concentrations of O_2 and H_2O < 0.1 ppm or oven-dried glassware (at 100 ºC overnight and cooled under vacuum prior use) using Schlenk techniques under argon atmosphere (otherwise mentioned).
NMR spectra were obtained on a Bruker 400 MHz, a 500 MHz or a 500 MHz with cryoprobe spectrometers equipped with probeheads capable of producing gradients in the z direction with a maximum strength of 53.5 G cm^{-1}. ^{1}H, ^{13}C, ^{19}F and ^{31}P NMR chemical shifts are reported in parts per million (ppm), relative to tetramethylsylane (TMS) for ^{1}H and ^{13}C with the residual solvent peak used as an internal reference, relative to $CFCl_3$ (Freon) for ^{19}F and relative to 85% H_3PO_4 for ^{31}P. In the ^{19}F and ^{31}P NMR spectra registered in non-deuterated solvents, a coaxial tube containing acetone-d_6 or dimethylsulfoxide-d_6 was used to maintain the lock ^{2}H signal. Multiplicities are reported as follows: singlet (s), doublet (d), broad doublet (bd), doublet of doublets (dd), doublet of quadruplets (dq), triplet (t), quadruplet (q), doublet of quadruplet of quadruplets (dqq) and multiplet (m). ^{19}F NMR yields for stoichiometric reductive elimination studies were obtained on a Bruker 400 MHz spectrometer using fluorobenzene (–113.4 ppm) or 4,4´-difluorobenzene (–116.8 ppm) as an internal standard with 32 scans for data acquisition. All diffusion ^{1}H and ^{19}F NMR experiments were carried out on dilute solutions (about 2 mg of product dissolved in 0.6 mL of the corresponding solvent for compound **4**) at 25 ºC to minimize the effect of different solution viscosities for different samples, which were confirmed from the diffusion coefficient value of the residual solvent signal taken as internal reference. To check for the presence and effective suppression of deleterious convection effects, a test LEDBP experiment was recorded for the first sample with and without sample rotation, and the results were compared to data obtained from double-stimulated echo sequence.[1] Thus, we decided to run DOSY experiments for all samples using the double-stimulated echo sequence incorporating bipolar gradient pulses and a longitudinal eddy current delay (dstegp3s in the Bruker library) and without sample rotation. The gradient strength was linearly incremented in 16 steps from 2% up to 95% of the maximum gradient strength. Diffusion times and gradient pulse durations were optimized for each experiment in order to achieve a 95% decrease in the resonance intensity at the largest gradient amplitude; typically, diffusion times (Δ) of 150 ms and bipolar rectangular gradient pulses (δ) of 1.0 were employed. The longitudinal eddy current delay was held constant to 5 ms, whereas the gradient pulse recovery time was set to 100 µs. Data were processed with the standard DOSY program included into the Bruker TOPSPIN software package. The accuracy of the measurements was confirmed by obtaining the same experimental ^{1}H and ^{19}F diffusion coefficient value from two different ^{1}H and ^{19}F measurements of same NMR sample. The estimation of the hydrodynamic radius was performed according to the Stokes-Einstein equation using the viscosities values of 0.0006 kg/m·s (THF), 0.00046 kg/m·s (benzene) and 0.00079 kg/m·s (DMF) at 25 ºC.[2]

High Resolution Mass Spectrometry (HRMS) data was recorded on a LCT-Premier (Waters) or a MicroTOF Focus (Bruker Daltonics) mass spectrometers using ESI ionization technique and dichloromethane or tetrahydrofuran as solvent.
The details for the X-ray structure determination can be found in page S88.

Materials and Methods

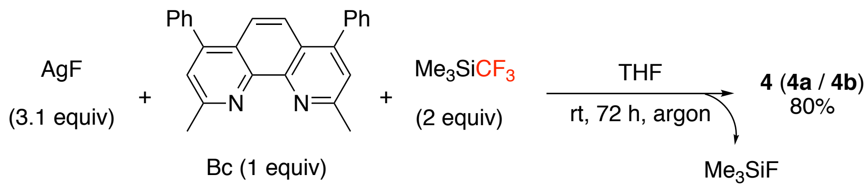
Commercially available reagents AgF, AgOAc, Ag_2O, $AgSbF_6$, CsF, KF, NBu_4OAc, Bathocuproine (Bc), Bathophenantroline, 1,3-Diisopropylimidazolinium chloride (SIPr·HCl), iodobenzene, fluorobenzene, 4,4´-difluorobiphenyl, Me_3SiCF_3, Et_3SiCF_3, $PhenCuCF_3$, $Pd(PPh_3)_4$, $Pd(dba)_2$, 1,3-Bis(diphenylphosphino)propane (dppp) and Xantphos were used without further purification directly as received from the commercial supplier, and stored under inert gas and/or low temperature when required.
If necessary, the solvents (Hexane, THF, CH_2Cl_2, toluene, Et_2O) were used from a solvent purification system *pure-solv* (SPS-400, Innovative Technology) and stored under argon over activated 4 Å molecular sieves. Anhydrous benzene and cyclohexane were used without further purification
Deuterated solvents (C_6D_6, THF-d_8, DMF-d_7, CD_2Cl_2) were stored under argon over activated molecular sieves 4 Å.
(Xantphos)Pd(Ph)I[3], (dppp)Pd(Ph)I[4] and SIPrAgCl[5] were synthesized according to previous literature procedures.
All the silver complexes are light-sensitive, so the reactions are performed in the dark to be preserved from light to avoid photodecomposition.

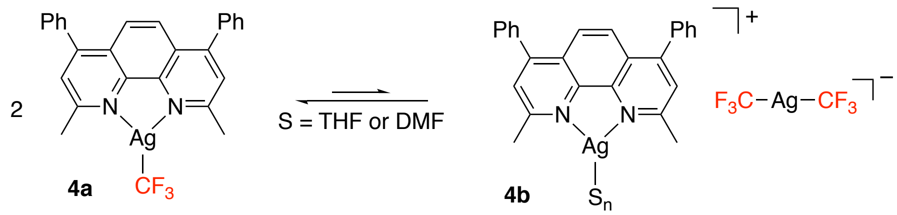
Modified Synthesis of 3



Complex **3** was prepared by a modification of the reported procedure.[6]
In an argon atmosphere glovebox, SIPrAgCl[5] (100 mg, 0.18 mmol) and NaO^{t}Bu (90.0, 0.9 mmol) were added to an oven-dried schlenk and 20 mL of THF were added. A solution of Me_3SiCF_3 (67 μL, 0.45 mmol) in THF (5 mL) was added dropwise and the solution was stirred 2 h at room temperature outside the glovebox. After that, the solution was filtered through a celite pad and the solvent was removed under reduced pressure. The residue was precipitated in a mixture of THF: hexane (1 mL: 15 mL) and the white solid was dried under vacuum to afford **3**. Yield: (95.7 mg; 90%).
The ^{1}H and ^{19}F NMR spectra are in accordance with the previously reported one.[6]
The complex must be stored at –30 ºC under inert atmosphere to avoid decomposition.

Synthesis and characterization of 4 (4a/4b)





In an argon atmosphere glovebox, AgF (130 mg, 1.02 mmol) and Bathocuproine (173 mg, 0.48 mmol) were added to an oven-dried schlenk containing a magnetic stir bar. The schlenk was capped with a septum. THF (30 mL) was added and the mixture was stirred at room temperature for 30 min. In parallel, a solution of Me_3SiCF_3 (0.15 mL, 1.0 mmol) in THF (5 mL) was prepared and it was added dropwise to the silver suspension and the mixture was stirred for 24 h. After that, the solution was filtered through cannula to other schlenk with AgF (65 mg, 0.51 mmol) previously weighted in the glovebox. The solution was left stirring for 48 h at room temperature. After that, the solution was filtered through cannula and the solvent was removed under reduced pressure. The solid residue was washed with hexane (2 x 10 mL) and the white-yellow solid was dried under vacuum to afford **4** (206.3 mg, 80% yield). The complex can be stored indefinitely at –30 ºC under inert atmosphere in the dark for months without any sign of decomposition.

Characterization in THF

^{1}H NMR (500 MHz, THF-d_8, 25 ºC): δ 7.82 (s, 2H), 7.68 (s, 2H), 7.58–7.49 (m, 10H), 3.03 (s, 6H).

^{13}C NMR (126 MHz, THF-d_8, 25 ºC): δ 159.72, 150.63, 145.88, 139.01, 130.67, 129.65, 125.80, 125.51, 124.07, 27.01. No signal for *C*F_3 was observed due to the low signal-to-noise ratio.

^{19}F NMR (470 MHz, THF-d_8, 25 ºC): δ –21.84 (2d, $^2J_{109Ag,F}$ = 122.3 Hz, $^2J_{107Ag,F}$ = 107.0 Hz, **4a**), –27.18 (2d, $^2J_{109Ag,F}$ = 100.7 Hz, $^2J_{107Ag,F}$ = 87.2 Hz, **4b**).

HRMS-electrospray (-) in tetrahydrofuran (m/z): $[M]^-$ calcd for C_2AgF_6, 244.8955 and 246.8952; found 244.8962 and 246.8965.

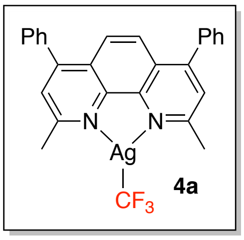
Characterization in DMF

^{1}H NMR (500 MHz, DMF-d_7, 25 ºC): δ 7.97 (s, 2H),7.86 (s, 2H), 7.73–7.60 (m, 10H), 3.02 (s, 6H).

^{13}C NMR (126 MHz, DMF-d_7, 25 ºC): δ 160.15, 151.78, 143.80, 138.12, 130.95, 130.33, 130.10, 126.82, 126.25, 124.78, 28.20. No signal for *C*F_3 was observed due to the low signal-to-noise ratio.

^{19}F NMR (470 MHz, DMF-d$_7$, 25 ºC): δ –19.19 (broad, **4a**), –24.98 (2d, $^2J_{109Ag,F}$ = 98.7 Hz, $^2J_{107Ag,F}$ = 84.6 Hz, **4b**).

Characterization in benzene



^{1}H NMR (500 MHz, benzene-d$_6$, 25 ºC): δ 7.52 (s, 2H), 7.31–7.10 (m, 10H, overlapping peaks with C_6D_6), 6.93 (s, 2H), 2.81 (s, 6H, CH_3).

^{13}C NMR (126 MHz, benzene-d$_6$, 25 ºC): δ 158.61, 148.55, 146.48, 138.85, 129.98, 128.68, 128.35, 124.96, 124.03, 123.17, 26.10. No signal for $\mathit{C}F_3$ was observed due to the low signal-to-noise ratio.

^{19}F NMR (470 MHz, benzene-d$_6$, 25 ºC): δ –19.24 (bd).

Unfruitful synthesis of (Bathophenanthroline)Ag(CF_3)

In our hands, the protocol for synthesizing (Bathophenanthroline)Ag(CF_3)[7] also afforded similar $[Ag(CF_3)_2]^-$ species to complex **4b** and unidentified compounds.

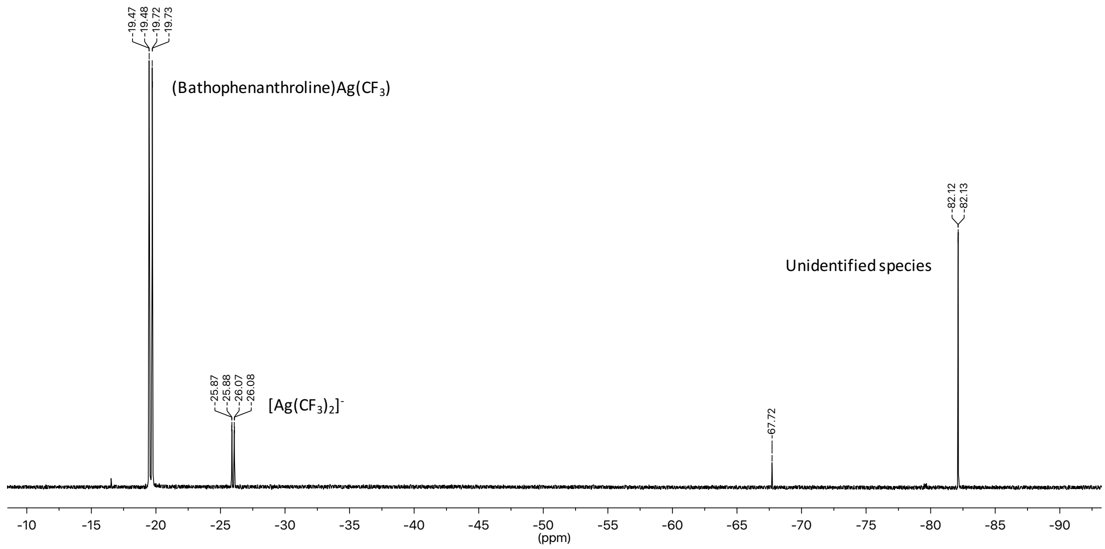


Figure S1. ^{19}F NMR spectrum of (Bathophenanthroline)Ag(CF_3) at 25 ºC in THF-d_8 at room temperature.

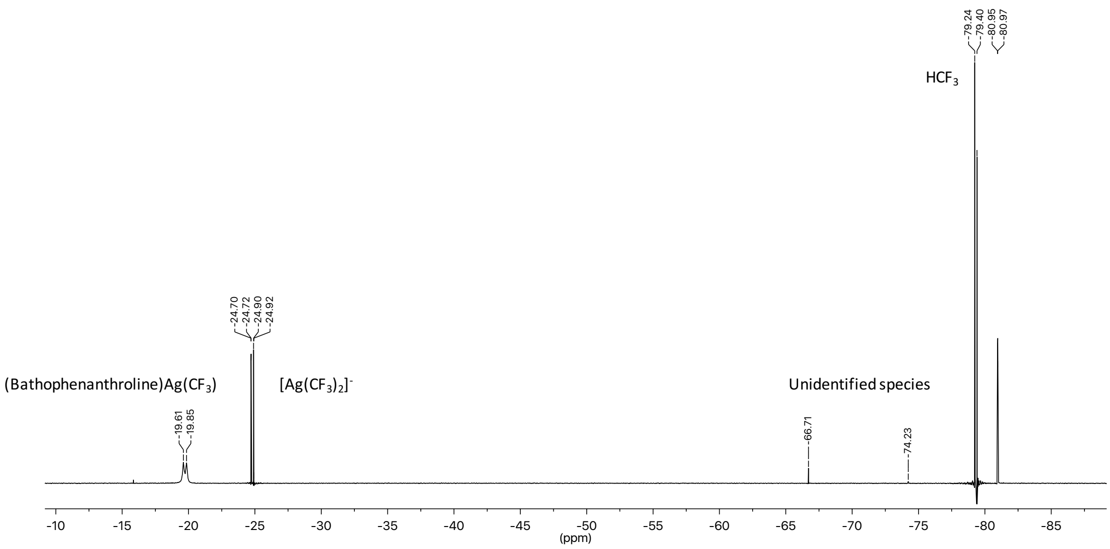
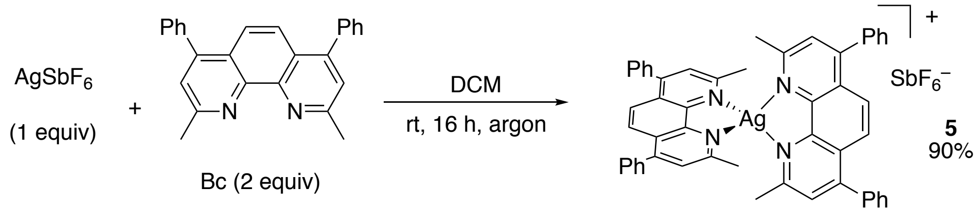


Figure S2. ^{19}F NMR spectrum of (Bathophenanthroline)Ag(CF_3) at 25 ºC in DMF-d_7 at room temperature.

Synthesis and characterization of 5



In an argon atmosphere glovebox, $AgSbF_6$ (50 mg, 0.15 mmol) and Bathocuproine (108 mg, 0.30 mmol) were added to an oven-dried schlenk containing a magnetic stir bar. DCM (50 mL) was added and the mixture was stirred at room temperature overnight. After that, the solution was filtered through cannula and the mixture was concentrated to 5 ml and hexane was added to precipitate the product. The solid residue was washed with hexane (2 x 10 mL) and the white solid was dried under vacuum to afford **5** (144 mg, 90% yield).

Characterization in DCM

^{1}H NMR (500 MHz, CD_2Cl_2, 25 ºC): δ 8.00 (s, 4H), 7.75 (s, 4H), 7.66–7.55 (m, 20H), 2.89 (s, 12H).

^{13}C NMR (126 MHz, CD_2Cl_2, 25 ºC): δ 158.66, 151.62, 143.53, 137.57, 130.12, 129.78, 129.50, 126.25, 125.85, 124.40, 28.25.

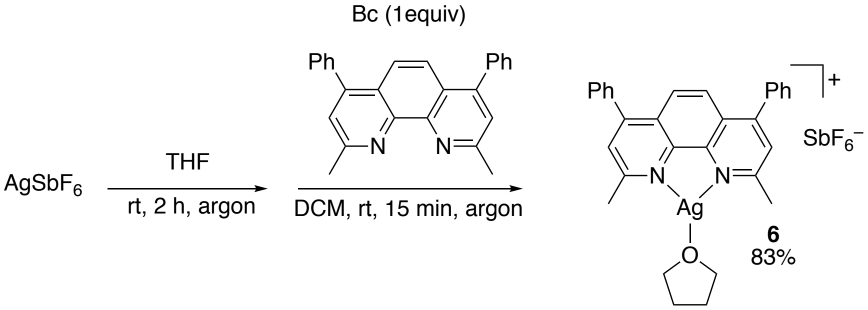
HRMS-electrospray in dichloromethane (m/z): $[M]^+$ calcd for $C_{52}H_{40}AgN_4$, 827.2304 and 829.2301; found 827.2319 and 829.2337.

Characterization in THF

^{1}H NMR (500 MHz, THF-d_8, 25 ºC): δ 8.05 (s, 4H), 7.92 (s, 4H), 7.69–7.54 (m, 20H), 2.94 (s, 12H).

^{13}C NMR (126 MHz, THF-d_8, 25 ºC): δ 159.45, 151.79, 143.64, 137.95, 130.35, 129.78, 129.53, 126.28, 126.16, 124.46, 27.73.

Synthesis and characterization of 6

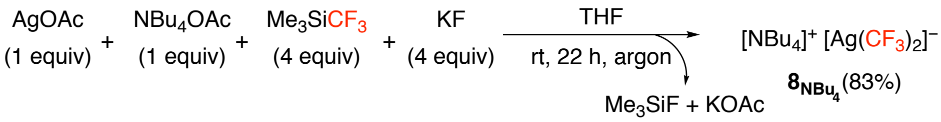


In an argon atmosphere glovebox, $AgSbF_6$ (10 mg, 0.029 mmol) was dissolved in 10 mL of THF and the solution was stirred for 2 hours at room temperature. To this solution was added a solution of Bathocuproine (10.4 mg, 0.029 mmol) in 1 mL of CH_2Cl_2 and the mixture was stirred 15 min at room temperature. Then, the mixture was concentrated to 1 mL and hexane was added to precipitate the product. The white solid was washed with hexane (2 x 5 mL) and it was dried under vacuum at low temperature to yield **6** (13 mg, 83% yield). The complex was stored at –32 ºC to avoid decomposition. We observe the formation of complex **6** after exposure of complex **5** to THF by single crystal X-ray diffraction.

^{1}H NMR (500 MHz, CD_2Cl_2, 25 ºC): δ 7.92 (s, 2H), 7.76 (s, 2H), 7.62–7.56 (m, 10H), 3.83 (m, 4H, THF), 3.03 (s, 6H, CH_3), 1.90 (m, 4H, THF).

^{13}C NMR (126 MHz, CD_2Cl_2, 25 ºC): 158.66, 152.10, 142.75, 137.40, 130.13, 129.63, 129.36, 126.24, 126.07, 124.41, 69.74, 28.77, 26.15.

Synthesis and characterization of $\mathbf{8_{NBu_4}}$



In an argon atmosphere glovebox, a schlenk was charged with AgOAc (50 mg, 0.29 mmol), NBu_4OAc (90.3 mg, 0.29 mmol) and KF (67.4 mg, 1.16 mmol) and dissolved in 20 mL of THF. A solution of Me_3SiCF_3 (171.5 µL, 1.16 mmol) in 10 ml of THF was added and this mixture was stirred 22 h until the signal at –21.40 (2d, $^2J_{109Ag,F}$ = 132.8 Hz, $^2J_{107Ag,F}$ = 115.1 Hz) ppm corresponding of $(NBu_4)[Ag(CF_3)(OAc)]$ had completely disappeared. The white suspension was filtered of at –20 ºC and the solution was then reduced to dryness under vacuum at this temperature. The white oil was recrystallized in a mixture of cold THF (1 mL) and cold hexane (20 mL) affording a crystalline white solid (120 mg, 83% yield). It was stored inside the glovebox at –32 ºC to avoid decomposition.

^{1}H NMR (500 MHz, DMF-d_7, 25 ºC): δ 3.25 (m, 8H, NCH_2), 1.70 (m, 8H, NCH_2CH_2), 1.43 (m, 8H, $NCH_2CH_2CH_2$), 1.02 (t, $^3J_{H,H}$= 7.4 Hz,12H, CH_3).

^{13}C NMR (126 MHz, DMF-d_7, 25 ºC): δ 155.85 (dqq, $^1J_{C,109Ag}$ = 257.0 Hz, $^1J_{C,F}$ = 371.0 Hz, $^3J_{C,F}$ = 8.1 Hz), 155.70 (dqq, $^1J_{C,107Ag}$ = 257.0 Hz, $^1J_{C,F}$ = 371.0 Hz, $^3J_{C,F}$ = 8.1 Hz), 59.33 (broad triplet, NCH_2), 24.61 (s, NCH_2CH_2), 20.82 (broad triplet, 8H, $NCH_2CH_2CH_2$), 14.19 (s, CH_3).
In this particular case, the highly symmetric environment around ^{14}N allows the observation of the *J* couplings ^{13}C - ^{14}N.

^{19}F NMR (470 MHz, DMF-d_7, 25 ºC): –25.19 (2d, $^2J_{109Ag,F}$ = 100.5 Hz, $^2J_{107Ag,F}$ = 87.0 Hz) ppm.

HRMS-electrospray (-) in tetrahydrofuran (m/z): $[M]^-$ calcd for C_2AgF_6, 244.8955 and 246.8952; found 244.8950 and 246.8949.

Stability of complex $\mathbf{8_{NBu_4}}$

-Solid state
At room temperature, $\mathbf{8_{NBu_4}}$ starts to decompose into a brown solid. An analysis by ^{19}F NMR of the decomposed solid reveals the formation of Ag^{III} species[8] –31.68 (2d, $^2J_{109Ag,F}$ = 41.0 Hz, $^2J_{107Ag,F}$ = 35.6 Hz) ppm.

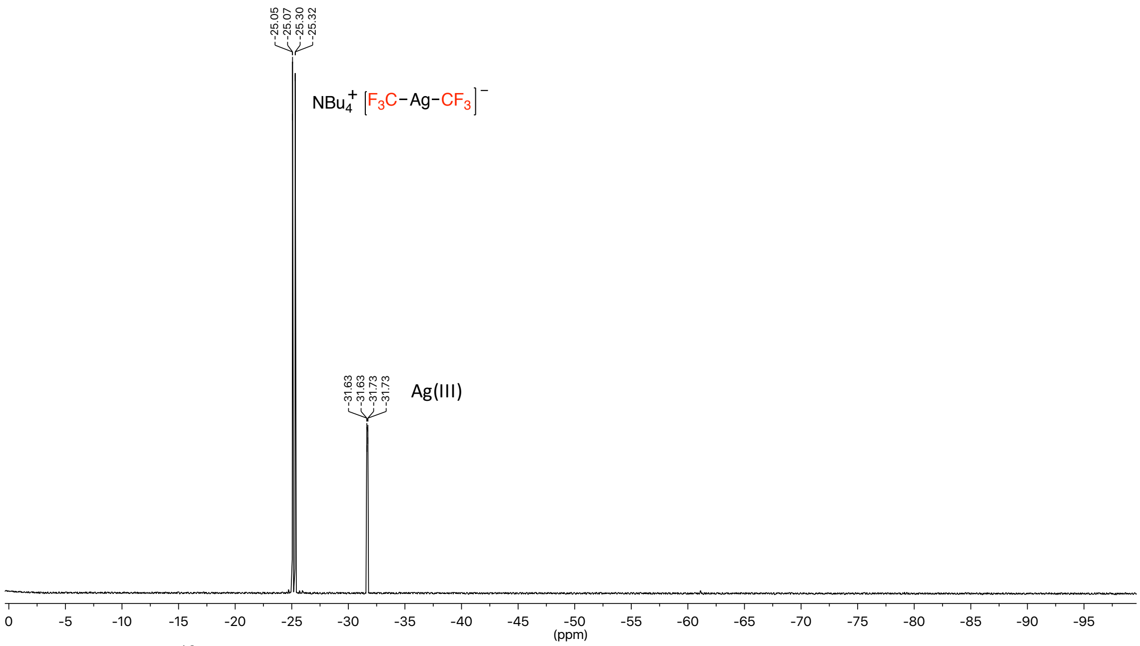


Figure S3. ^{19}F NMR spectrum of $\mathbf{8_{NBu_4}}$ at 25 ºC in THF (acetone-d6) after one day at room temperature

-Solution

Two different tests were carried out to check the stability of this salt in solution.

1) A J-young NMR tube was charged with $\mathbf{8_{NBu_4}}$ (2.9 mg, 0.006 mmol), dissolved in 0.6 mL of THF (0.01 M) and left standing at room temperature covered with aluminum foil to prevent photodecomposition. ^{19}F NMR spectra were acquired over the time and the mass percentage was determined by comparing the original mass of the sample to the number of moles of $\mathbf{8_{NBu_4}}$ determined by dissolving the sample and integrating its resonance in the ^{19}F NMR spectrum against approx. 5 mg of 4,4´-difluorobiphenyl added as standard. The solution of $\mathbf{8_{NBu_4}}$ in THF didn´t present any sign of decomposition during 7 days based of ^{19}F NMR spectra. After two months, the complex loses around 5% of its mass balance after one night with the appearance of HCF_3 and $[Ag(CF_3)_4]^-$ in the ^{19}F NMR spectra.

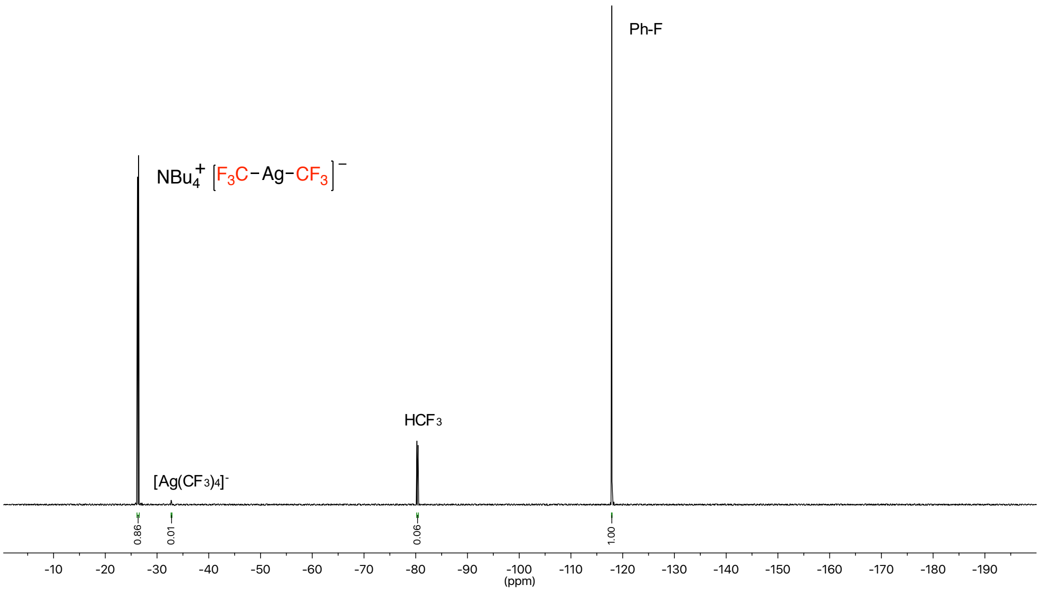


Figure S4. ^{19}F NMR spectrum of $\mathbf{8}_{\mathbf{NBu_4}}$ at 25 ºC in THF (acetone-d6) measured after two months at room temperature.

2) A J-young NMR tube was charged with $\mathbf{8}_{\mathbf{NBu_4}}$ (11.7 mg, 0.026 mmol), dissolved in 0.6 mL of THF (0.04 M), covered with aluminum foil to prevent photodecomposition and heated at 56 ºC. Mass percentage was determined by comparing the original mass of the sample to the number of moles of $\mathbf{8}_{\mathbf{NBu_4}}$ determined by dissolving the sample and integrating its resonance in the ^{19}F NMR spectrum against 10 mg of 4,4´-difluorobiphenyl added as standard.
The complex loses around 2% of its mass balance after one night with the appearance of HCF_3 in the ^{19}F NMR spectra.

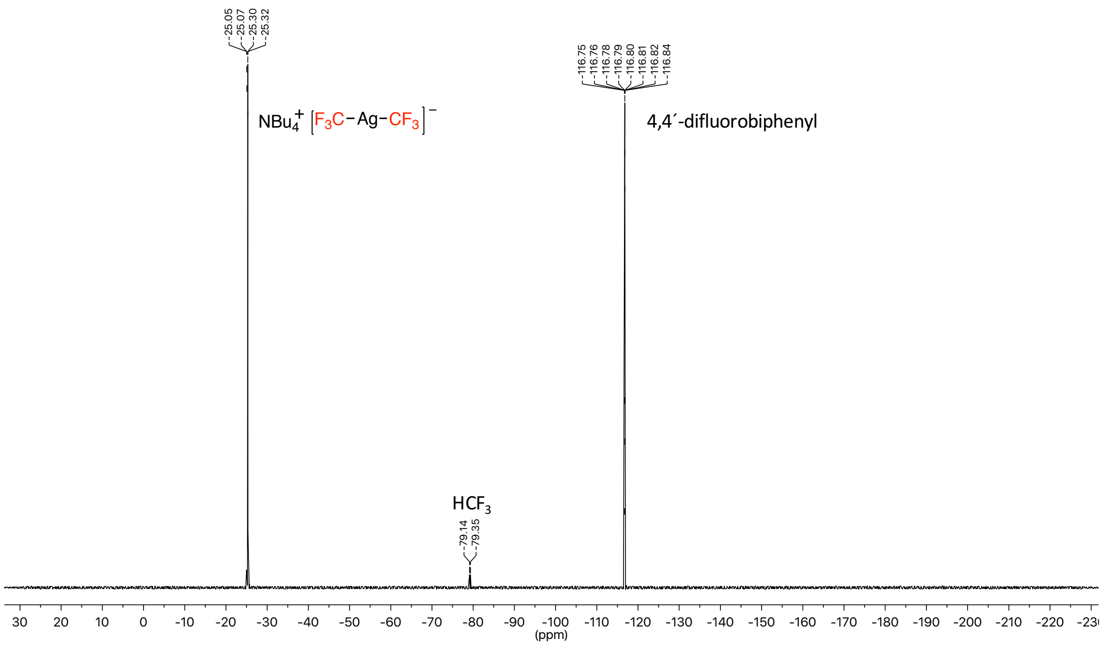
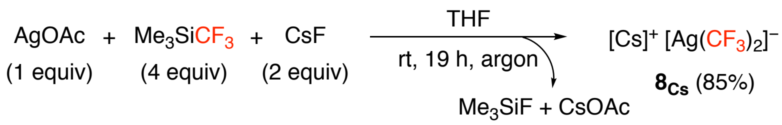


Figure S5. ^{19}F NMR spectrum of $\mathbf{8}_{\mathbf{NBu_4}}$ at 25 ºC in THF (acetone-d6) measured after one night at 56 ºC

Synthesis and characterization of 8_{Cs}



In an argon atmosphere glovebox, two duplicate reactions were carried out. The schlenks were charged equally with AgOAc (50 mg, 0.3 mmol) and CsF (73 mg, 0.49 mmol) and each one was dissolved in 30 mL of THF. A solution of Me_3SiCF_3 (142 μL, 1.04 mmol) in 10 mL of THF was added dropwise to each schlenk and the mixtures were stirred overnight. After 16 h, inside the glovebox, a schlenk was charged with CsF (108 mg, 0.71 mmol) and it was dissolved in 10 mL of THF. Outside the glovebox, each duplicate yellow suspension was filtered through cannula to the schlenk containing the CsF suspension and a solution of Me_3SiCF_3 (47 μL, 0.32 mmol) in 5 mL of THF was added dropwise to the schlenk. The mixture was stirred around 3 h until the reaction was completed and the signal of –21.15 ppm (2d, $^2J_{109Ag,F}$ = 133.4 Hz, $^2J_{107Ag,F}$ = 115.8 Hz) corresponding to $(Cs)[Ag(CF_3)(OAc)]$ had completely disappeared. At this point, the resulting yellow suspension was filtered through cannula at –20 ºC and the solution was then reduced to dryness under vacuum at this temperature. The yellow oily residue was recrystallized in a mixture of cold THF (1 mL) and cold hexane (20 mL) and the resulting yellow solid was washed with cold hexane (2 x 10 mL). The yellow solid (192 mg, 85% yield) was stored in the dark at –32 ºC to avoid decomposition.

^{13}C NMR (126 MHz, THF-d_8, 25 ºC): δ 154.10 (dqq, $^1J_{C,109Ag}$ = 256.5 Hz, $^1J_{C,F}$ = 371.6 Hz, $^3J_{C,F}$ = 7.5 Hz), 152.09 (dqq, $^1J_{C,107Ag}$ = 256.5 Hz, $^1J_{C,F}$ = 371.6 Hz, $^3J_{C,F}$ = 7.5 Hz) ppm.

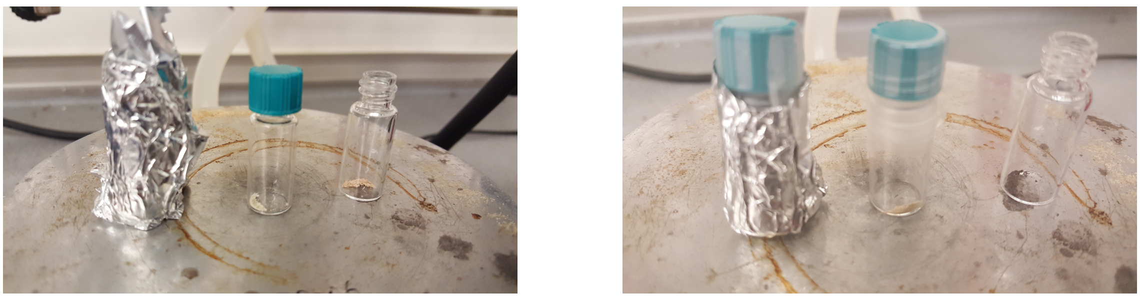
^{19}F NMR (470 MHz, THF-d_8, 25 ºC): –24.67 (2d, $^2J_{109Ag,F}$ = 98.6 Hz, $^2J_{107Ag,F}$ = 88.9 Hz) ppm.

HRMS-electrospray (-) in tetrahydrofuran (m/z): $[M]^-$ calcd for C_2AgF_6, 244.8955 and 246.8952; found 244.8970 and 246.8971.

Stability of complex 8_{Cs}

-Solid state

8_{Cs} decomposes under air conditions in less than 20 minutes, however it can be quickly weighted under air and afterwards purged under argon as soon as possible to prepare the corresponding reaction. On the other hand, under argon, it lasts one day at room temperature or non-protected from light. The black decomposed obtained residue is not soluble in common solvents and it is presumably metallic Ag.



15 min Next day

Figure S6. Stability of complex **8_{Cs}** in solid state.

-Solution

Two different tests were carried out to check the stability of this salt in solution.

1) A J-young NMR tube was charged with **8$_{Cs}$** (2.3 mg, 0.006 mmol), dissolved in 0.6 mL of THF (0.01 M) and left standing at room temperature covered with aluminum foil to prevent photodecomposition. ^{19}F NMR spectra were acquired over the time and the mass percentage was determined by comparing the original mass of the sample to the number of moles of **8$_{Cs}$** determined by dissolving the sample and integrating its resonance in the ^{19}F NMR spectrum against aprox. 5 mg of 4,4´-difluorobiphenyl added as standard.
The solution of **8$_{Cs}$** in THF didn´t present any sign of decomposition during 7 days based of ^{19}F NMR spectra. After two months, the complex loses around 15% of its mass balance after one night with the appearance of HCF_3 in the ^{19}F NMR spectra.

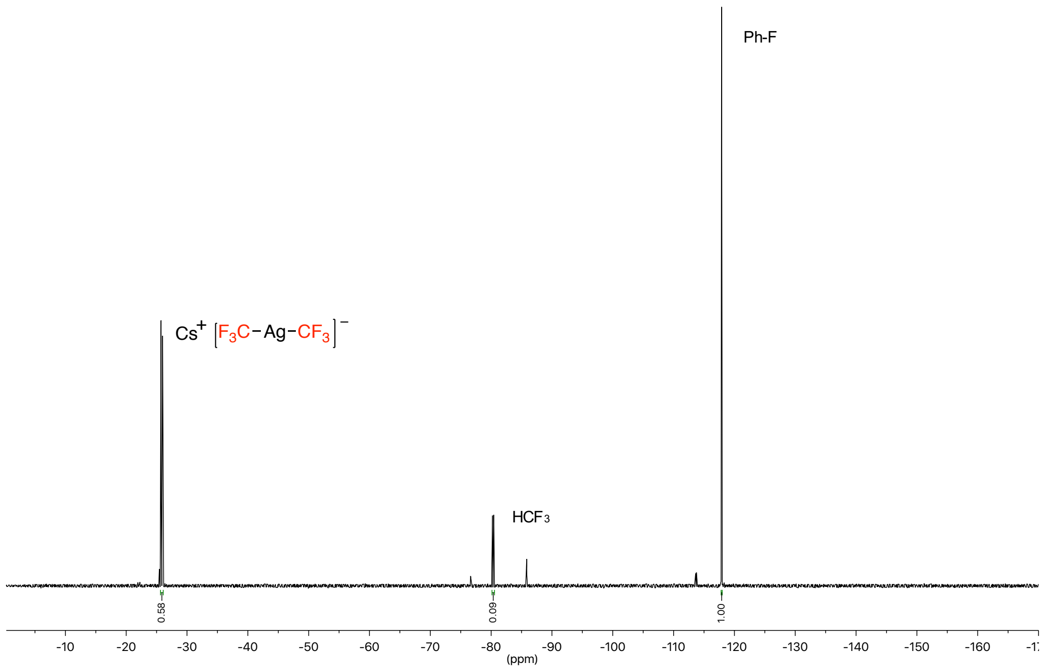


Figure S7. ^{19}F NMR spectrum of **8$_{Cs}$** at 25 ºC in THF (acetone-d$_6$) measured after two months at room temperature.

2) A J-young NMR tube was charged with **8$_{Cs}$** (10 mg, 0.026 mmol), dissolved in 0.6 mL of THF (0.04 M), covered with aluminum foil to prevent photodecomposition and heated at 56 ºC. Mass percentage was determined by comparing the original mass of the sample to the number of moles of **8$_{Cs}$** determined by dissolving the sample and integrating its resonance in the ^{19}F NMR spectrum against 10 mg of 4,4´-difluorobiphenyl added as standard.
The complex decomposes around 10% of its mass after one night at 56 ºC with the appearance of HCF_3 and presumably species related to $AgCF_2CF_3$ complexes resulted for α-fluorination elimination processes.

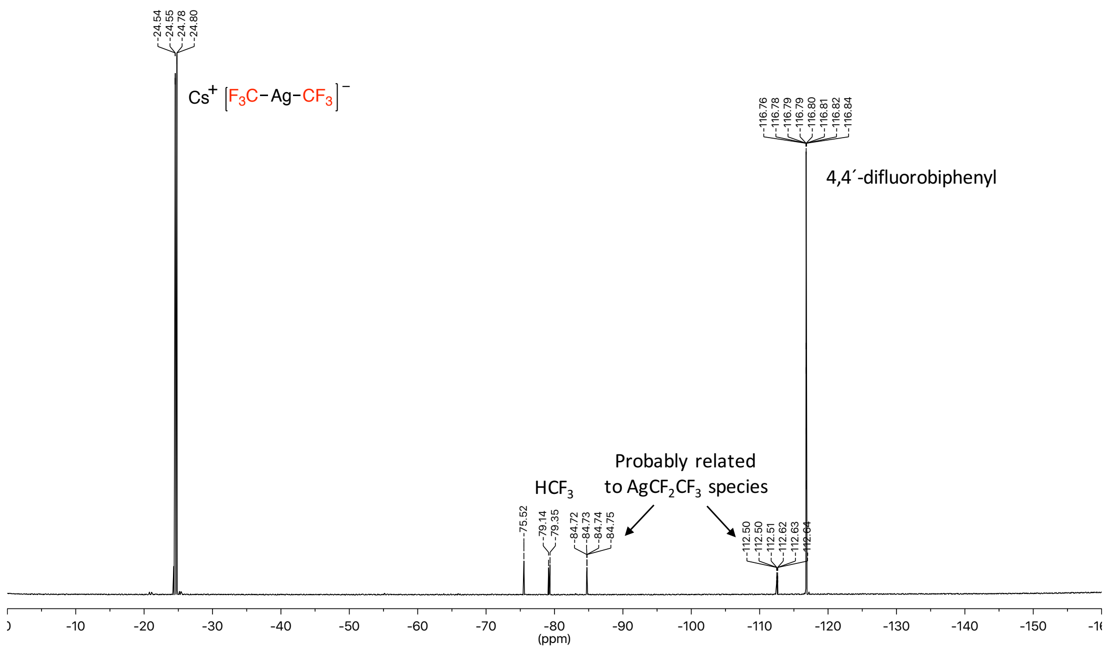


Figure S8. ^{19}F NMR spectrum of $\mathbf{8}_{\mathbf{Cs}}$ at 25 ºC in THF (acetone-d_6) measured after one night at 56 ºC

Investigation of the equilibrium between 4a and 4b

A) Solvent effect

To investigate the effect of solvent on the equilibrium between **4a** and **4b**, NMR samples of complex **4** (2 mg**,** 0.0037 mmol) in 0.6 mL of each solvent were prepared at room temperature inside the glovebox. The ratio between species **4a** and **4b** was taken directly by the integration of the corresponding ^{19}F NMR signals.

Table S1. Comparison of ratio between **4a** and **4b** by ^{19}F NMR at 0.0062 M

Ratio	Benzene-d6	THF-d8	DMF-d7
4a	100	98	66
4b	0	2	34

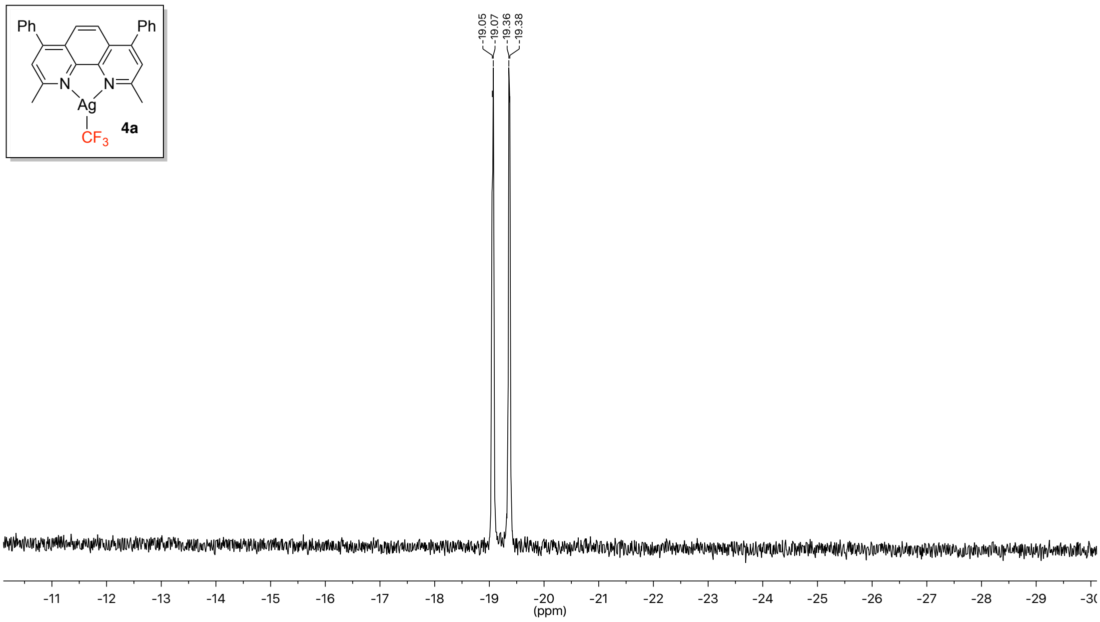


Figure S9. ^{19}F NMR spectrum of **4a** at 25 ºC at 0.0062 M (Benzene-d6)

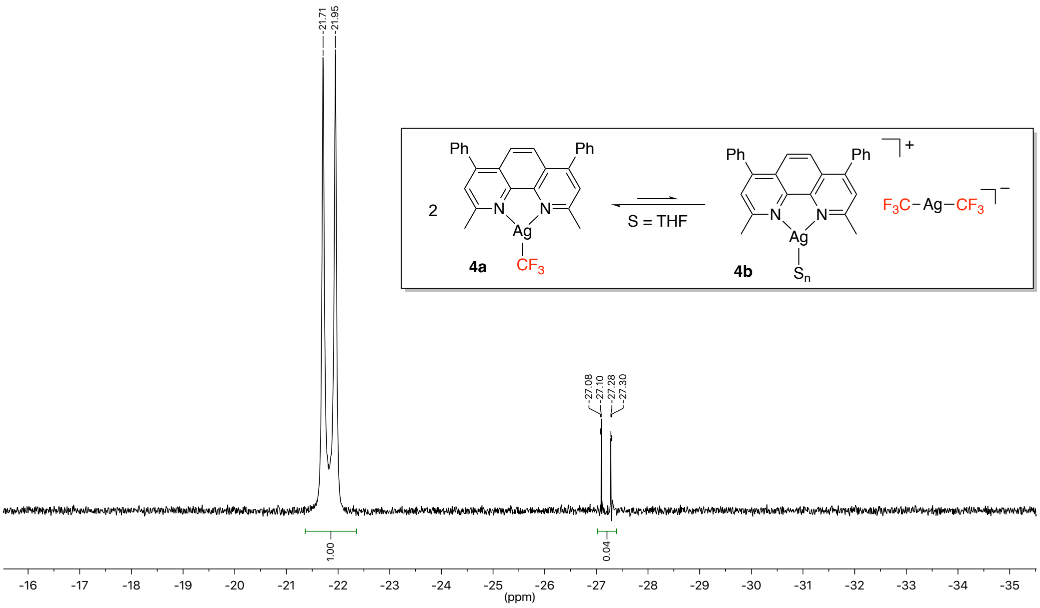


Figure S10. ^{19}F NMR spectrum of **4** at 25 ºC at 0.0062 M (THF-d8)

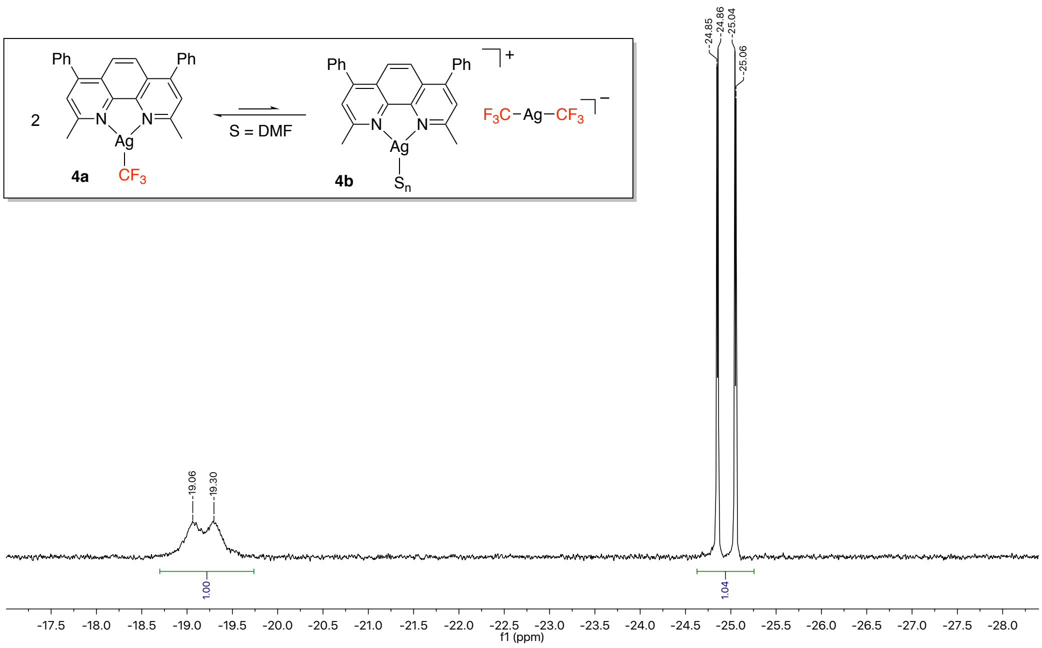


Figure S11. ^{19}F NMR spectrum of **4** at 25 ºC at 0.0062 M (DMF-d_7)

B) Temperature effect

Variable temperature NMR experiments were carried out in order to explore the behavior of the dynamic exchange between **4a** and **4b** at different temperatures for analyzing the splitting of the signals or the appearance of new ones if it was the case. For this, complex **4** (2 mg**,** 0.0037 mmol) was weighted inside the glovebox and dissolved in 0.6 mL of the corresponding solvent at room temperature. The ^{19}F NMR and ^{1}H NMR spectra were recorded from 25 ºC to –90 ºC in THF-d_8 or from 25 ºC to –40 ºC in DMF-d_7, and afterwards from the corresponding low temperature to 25 ºC again. In all the following figures, there are shown stacked plots of ^{19}F NMR and ^{1}H NMR spectra of compound **4** from 25 ºC to –90 ºC (THF-d_8) or –40 ºC (DMF-d_7). The spectra from low temperature to 25 ºC did not show any significant change. In all the cases, the pattern of the signals was maintained and no splitting or appearance of new signals was observed.

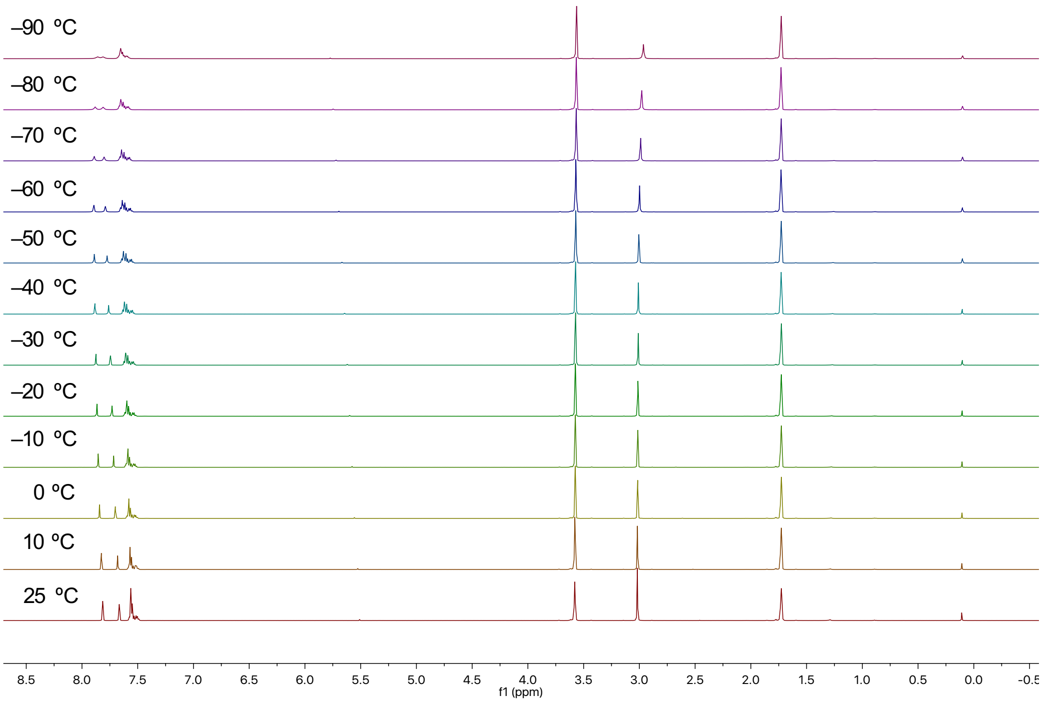


Figure S12. Variable temperature ^{1}H NMR spectrum of **4** (THF-d_8)

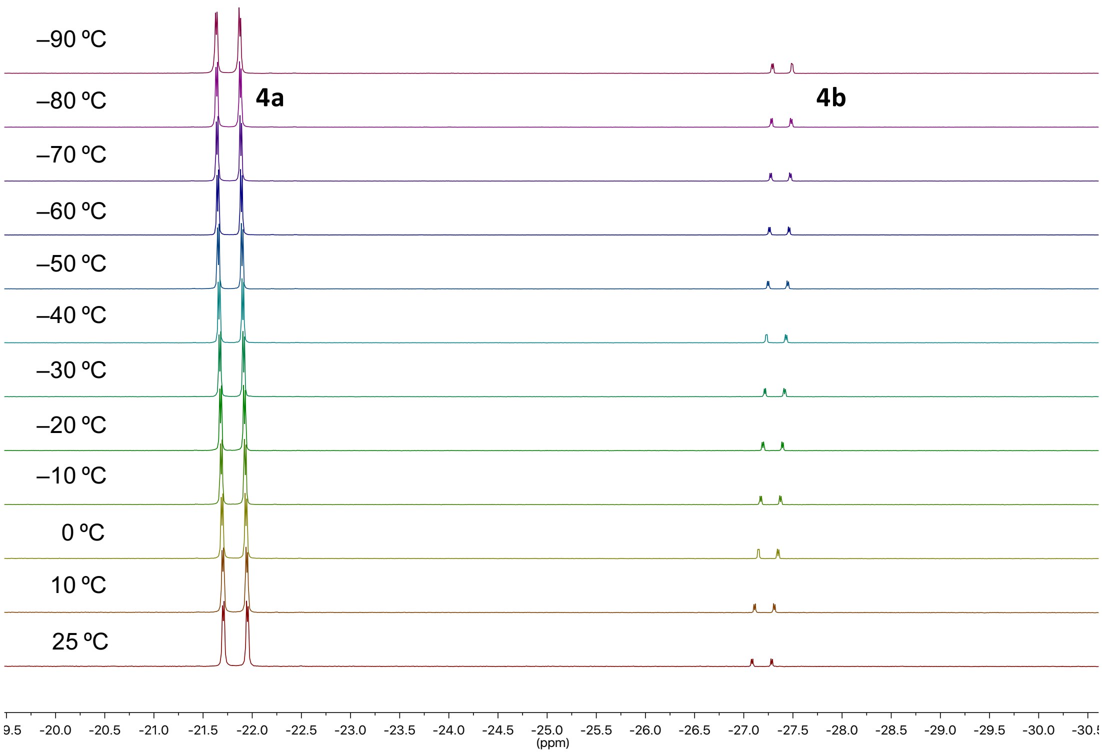


Figure S13. Variable temperature ^{19}F NMR spectrum of **4** (THF-d_8)

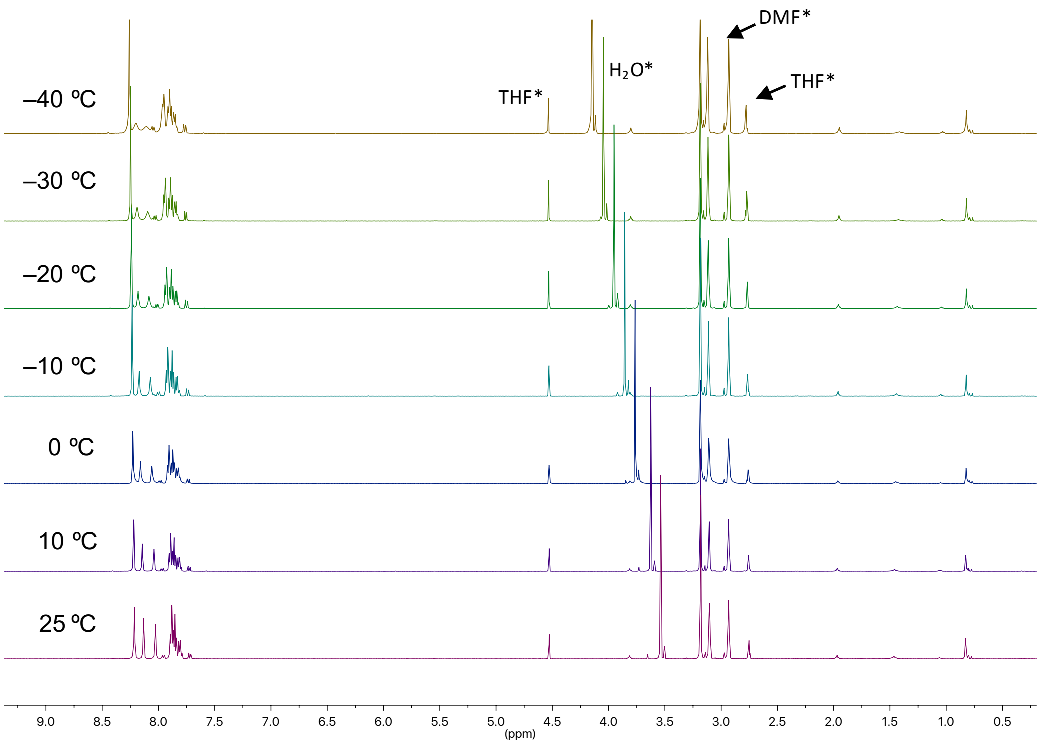


Figure S14. Variable temperature ^{1}H NMR spectrum of **4** (DMF-d$_7$)

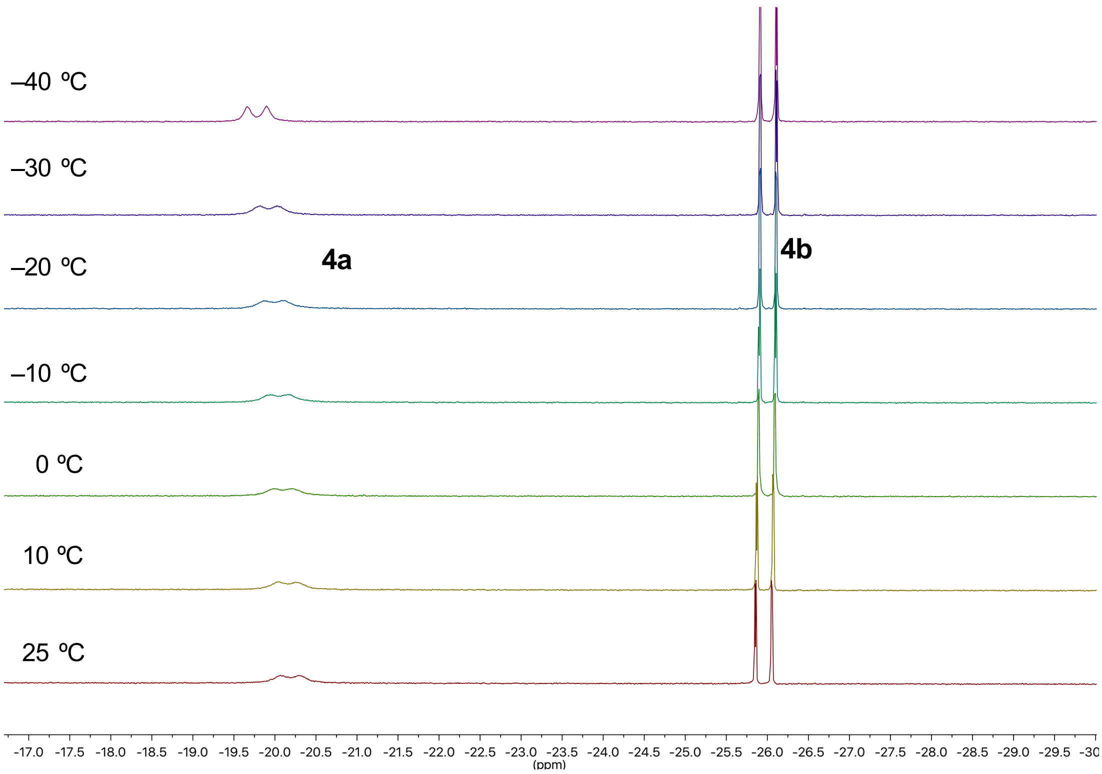


Figure S15. Variable temperature ^{19}F NMR spectrum of **4** (DMF-d$_7$)

We hypothesized that there are different regimes in the NMR time scale for the equilibrium between **4a** and **4b**. The rearrangement of the **Bc** ligands would be presumably involved in a fast-dynamic exchange process giving rise to one set of signals by ^{1}H NMR even at low temperature. On the other hand, the trifluoromethyl exchange reaction would probably take place in a slow-dynamic exchange process as observed by ^{19}F NMR spectra.

Diffusion-ordered 2D ^{1}H and ^{19}F NMR experiments (DOSY) of 4, 5 and Bc to investigate the nature of the cation of 4b, (Cation)$^{+}$[Ag(CF$_3$)$_2$]$^{-}$

The unexpected striking nature of the cation of **4b** prompts us to utilize diffusion-ordered 2D ^{1}H and ^{19}F NMR experiments. We envisioned that by measuring the diffusion coefficient (*D*) of the different species in solution and comparing them to targeted standards, it would be possible to unravel the structure of the non-intuitive cation of the ionic species in equilibrium with **4a**. For comparison purposes, the standards were selected based on their size and potential participation in the investigated equilibrium. We measured the diffusion coefficient, in THF and DMF, of Bathocuproine, along with **5**, $[(Bc)_2Ag]^{+}SbF_6^{-}$, as it contains independently the cation of the initially hypothesized $[(Bc)_2Ag]^{+}[Ag(CF_3)_2]^{-}$.

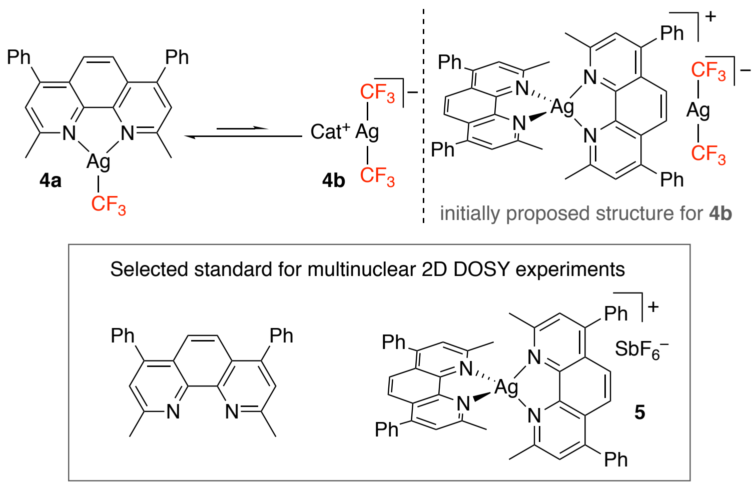


Figure S16. Chemical structures studied by DOSY experiments

The diffusion coefficients were measured in a logarithmic scale and the accuracy of the reported values is ± 0.01. The R_H values were obtained through the Stokes-Einstein equation (eq. S1) being K_B (Boltzmann constant), T (absolute temperature), η (viscosity) and D (diffusion coefficient).

$$D = \frac{K_B T}{6\pi\eta R_H} \qquad \text{(eq. S1)}$$

All diffusion ^{1}H and ^{19}F NMR experiments were carried out on dilute solutions (aprox. 0.0062 M for complex **4**) at 25 ºC to minimize the effect of different solution viscosities for different samples. The diffusion coefficient values were confirmed from the ones obtained for the residual solvent signal taken as internal reference, being these values approximately $D = 2.69 \cdot 10^{-9}$ m^2/s for benzene, $D = 3.16 \cdot 10^{-9}$ m^2/s for THF and $D = 1.66 \cdot 10^{-9}$ m^2/s for DMF.

Table S2. Comparison of diffusion coefficient (D) between free ligand (**Bc**), monomer complex (**4**) and dimer specie (**5**)

D (m^2/s)	**Bc**	**4a** ^{1}**H**	**4a** ^{19}**F**	**4b** ^{19}**F**	**5**
Benzene	$8.32\cdot10^{-10}$	$8.91\cdot10^{-10}$	$8.32\cdot10^{-10}$	x	$4.79\cdot10^{-10}$
THF	$1.10\cdot10^{-9}$	$1.10\cdot10^{-9}$	$1.15\cdot10^{-9}$	$1.41\cdot10^{-9}$	$6.92\cdot10^{-10}$
DMF	$6.31\cdot10^{-10}$	$5.62\cdot10^{-10}$	$6.31\cdot10^{-10}$	$1.26\cdot10^{-9}$	$4.07\cdot10^{-10}$

Table S3. Comparison of hydrodynamic radii (R_H) between free ligand (**Bc**), monomer complex (**4**) and dimer specie (**5**)

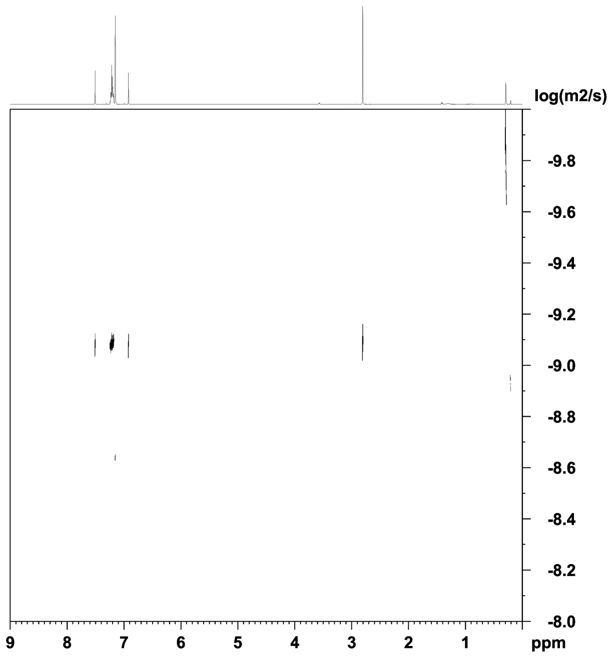
R_H (Å)	**Bc**	**4a** ^{1}**H**	**4a** ^{19}**F**	**4b** ^{19}**F**	**5**
Benzene	4.37	4.08	4.37	x	7.60
THF	4.33	4.33	4.13	3.36	6.86
DMF	4.38	4.91	4.38	2.14	6.78

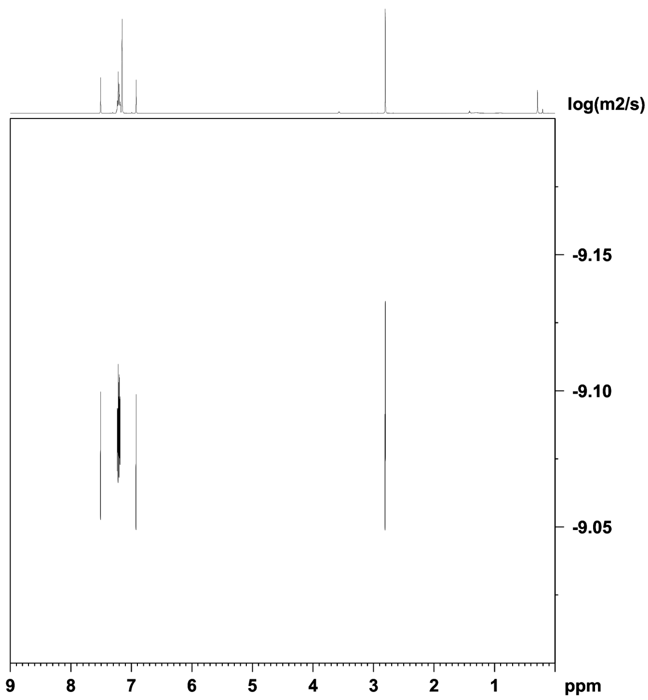
5 shows a significant larger R_h, by ^{1}H DOSY NMR, than the one obtained for the equilibrium mixture of **4a** and **4b**, in THF and DMF, assuming the shape of the molecule to be a sphere. This confirms the absence of a $[(Bc)_2Ag]^+$ as cation.

DOSY experiments in Benzene-d_6

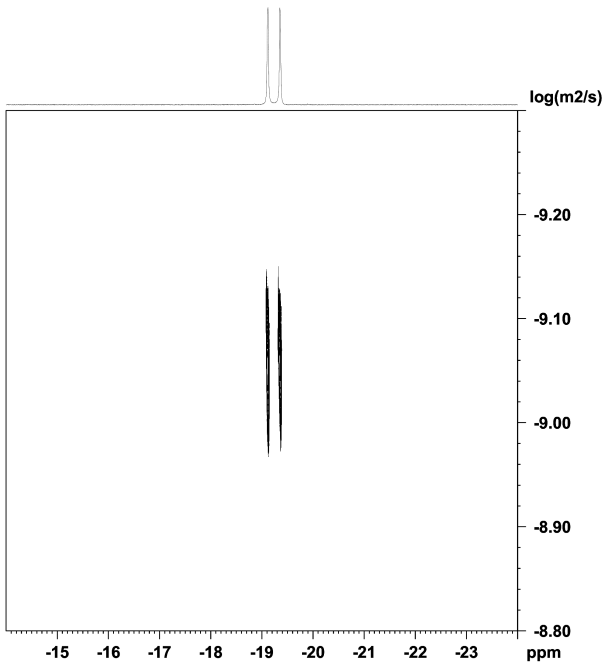
Spectra of 4

DOSY ^{1}H NMR spectrum of **4** at 25 °C (Benzene-d_6)



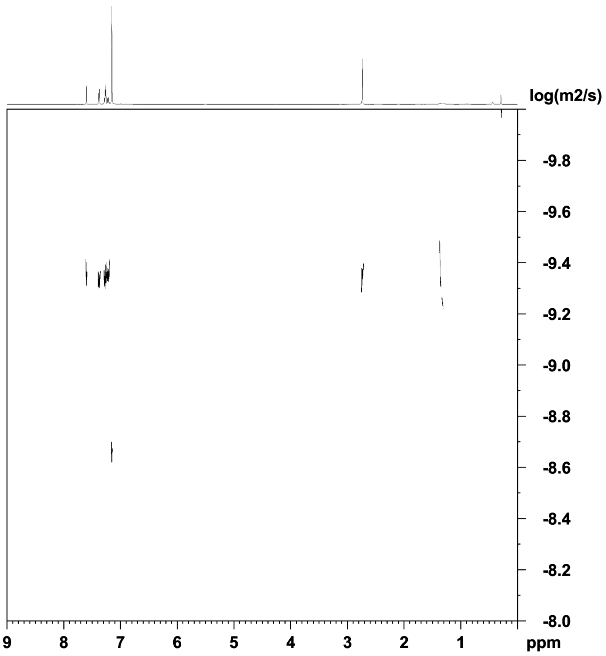


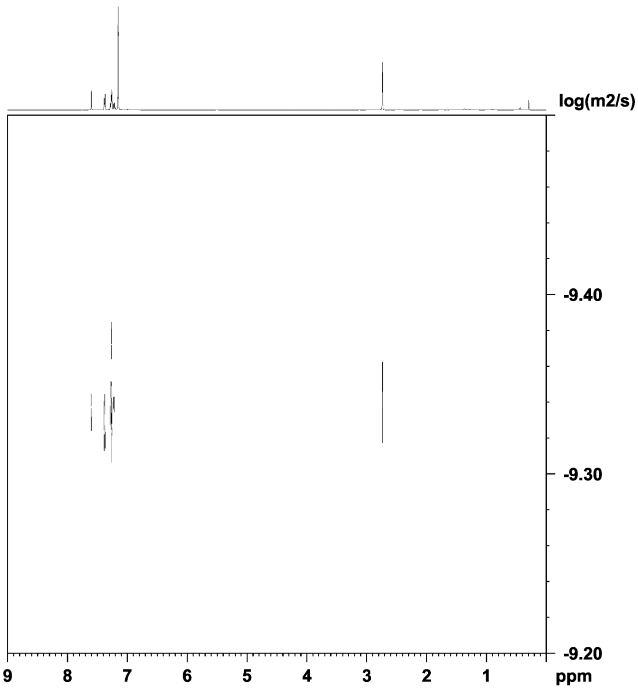
DOSY ^{19}F NMR spectrum of **4** at 25 ºC (Benzene-d_6)



Spectrum of 5

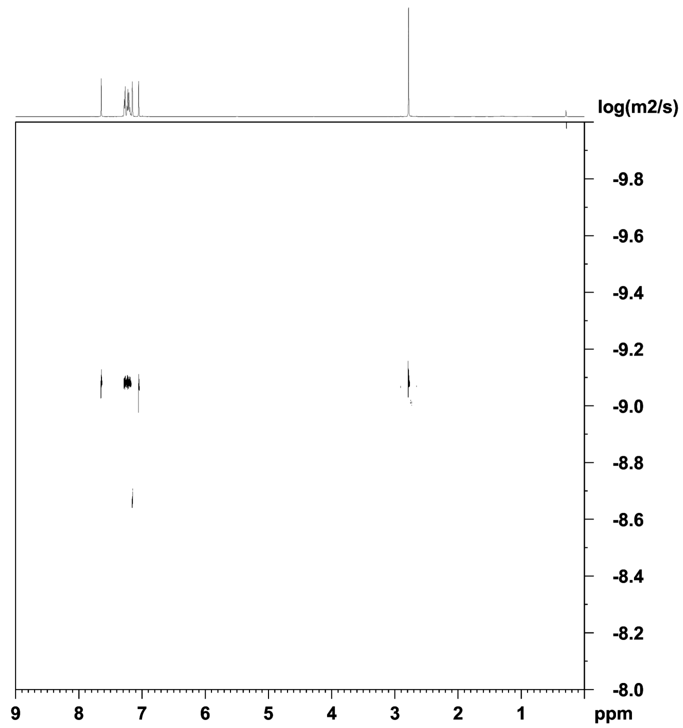
DOSY ^1H NMR spectrum of **5** at 25 ºC (Benzene-d_6)

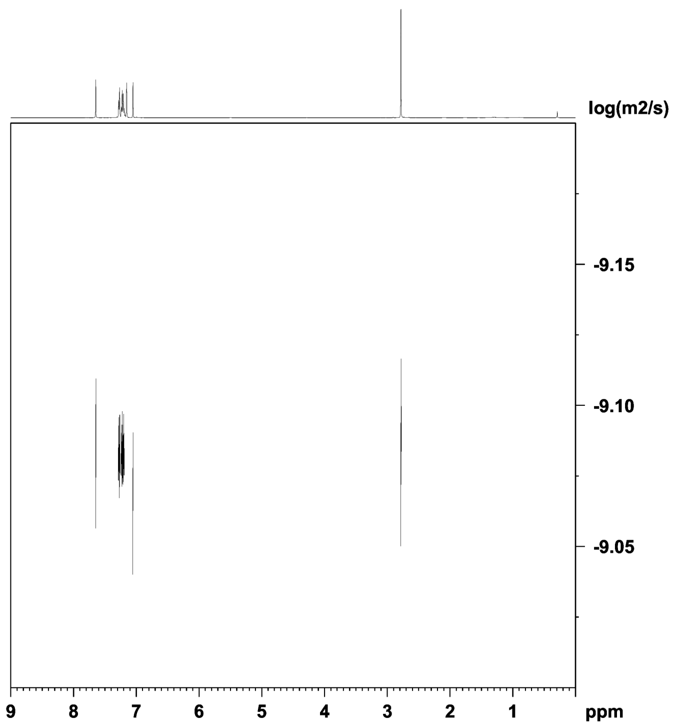




Spectrum of Bathocuproine (Bc)

DOSY ^{1}H NMR spectrum of **Bc** at 25 °C (Benzene-d_6)

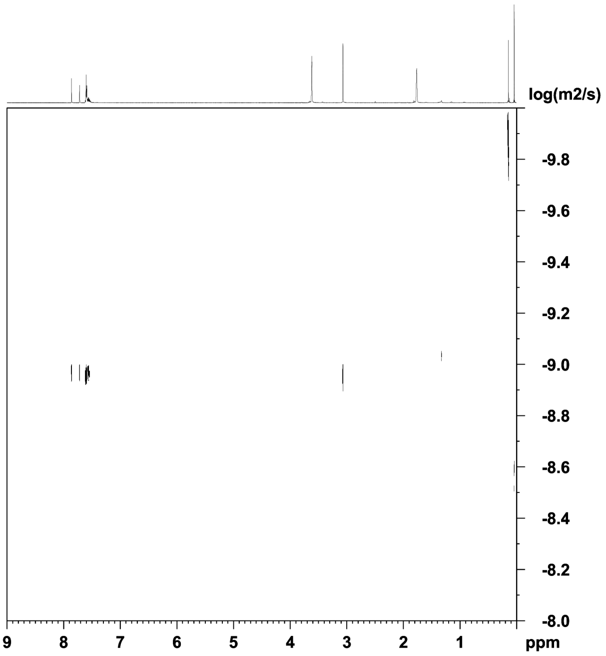




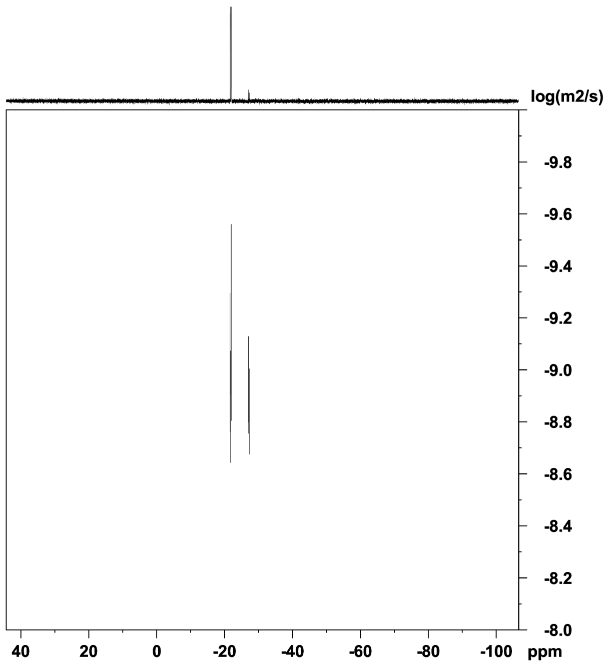
DOSY experiments in THF-d_8

Spectrum of 4

DOSY ^1H NMR spectrum of **4** at 25 °C (THF-d_8)

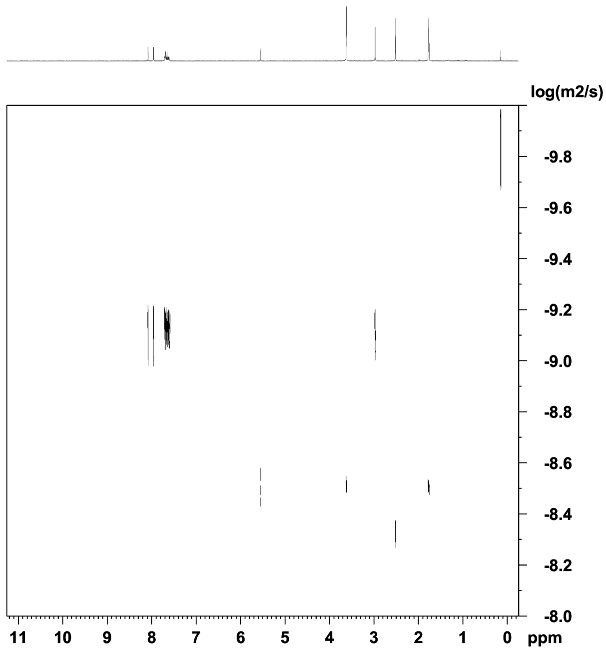


DOSY ^{19}F NMR spectrum of **4** at 25 °C (THF-d_8)



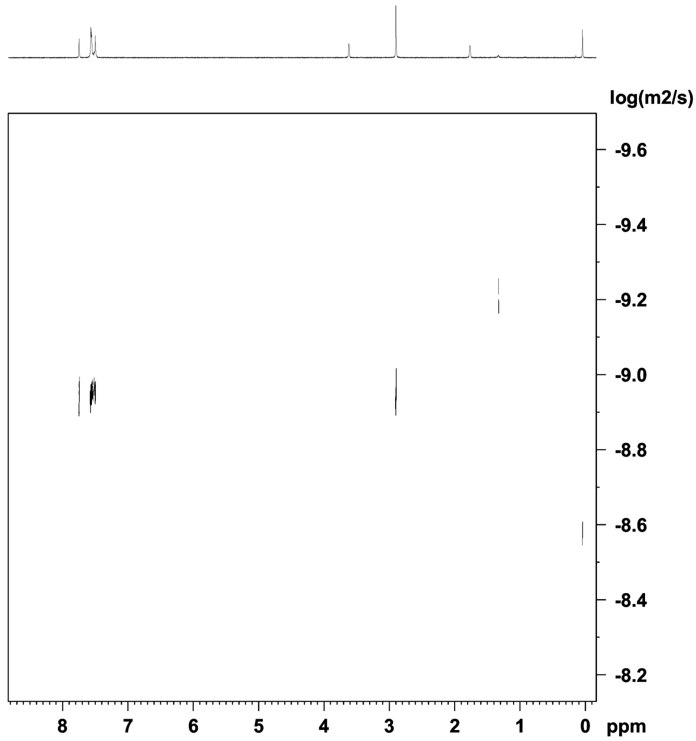
Spectrum of 5

DOSY ^1H NMR spectrum of **5** at 25 ºC (THF-d_8)



Spectrum of Bathocuproine (Bc)

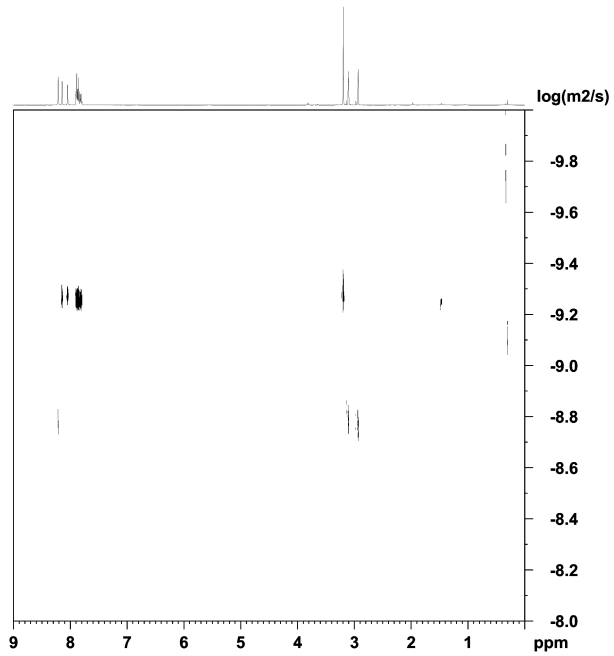
DOSY ^{1}H NMR spectrum of **Bc** at 25 ºC (THF-d_8)

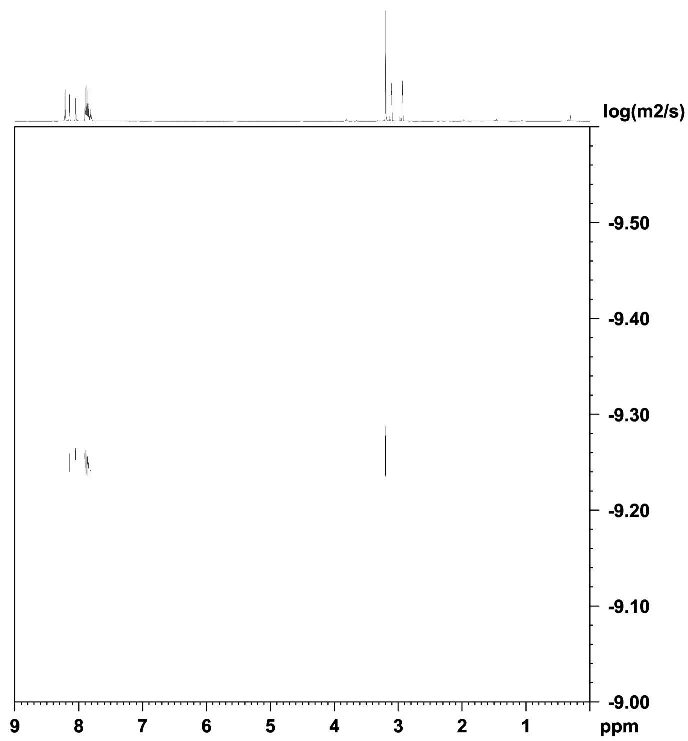


DOSY experiments in DMF-d_7

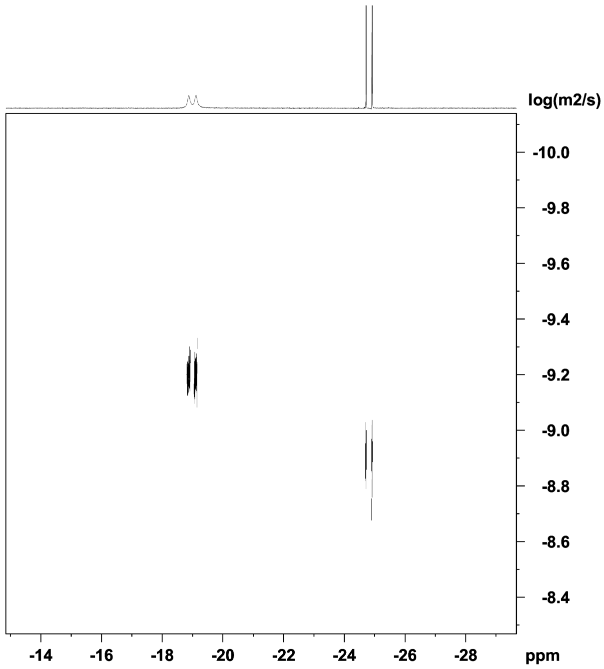
Spectra of 4

DOSY ^{1}H NMR spectrum of **4** at 25 °C (DMF-d_7)



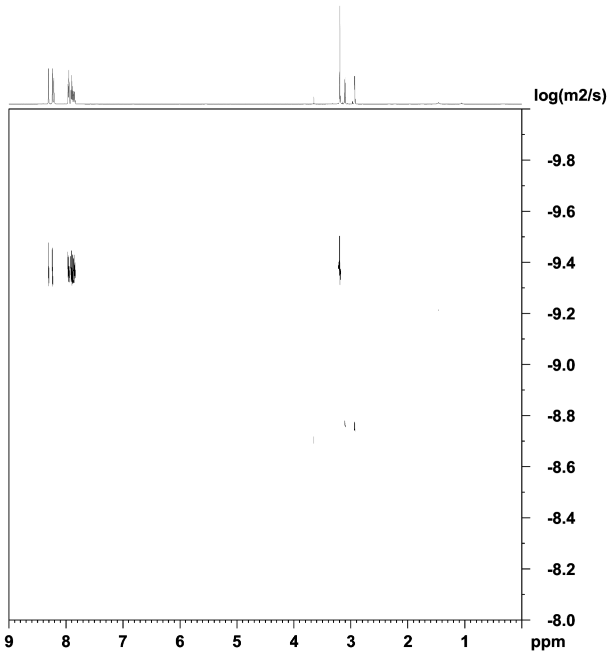


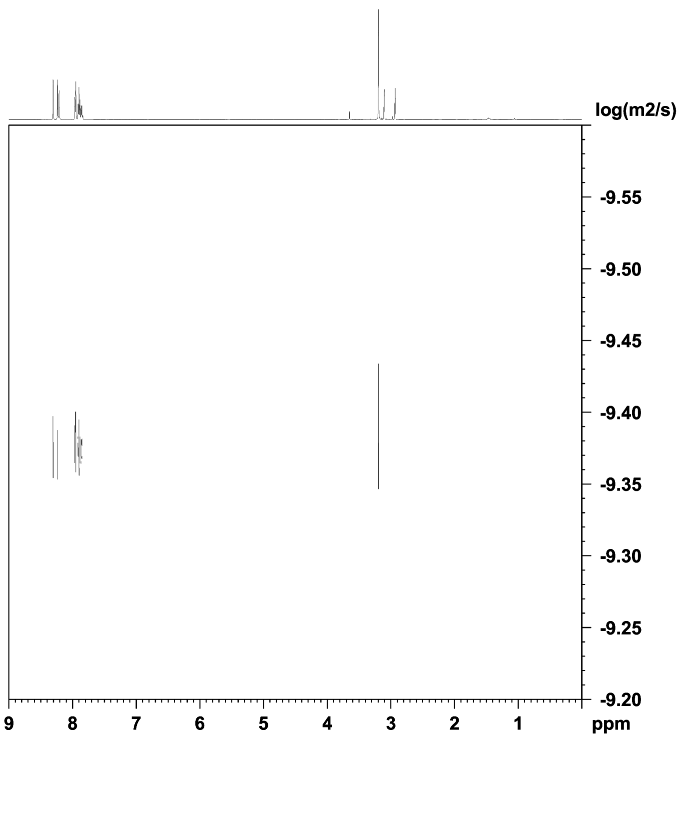
DOSY ^{19}F NMR spectrum of **4** at 25 ºC (DMF-d_7)



Spectrum of 5

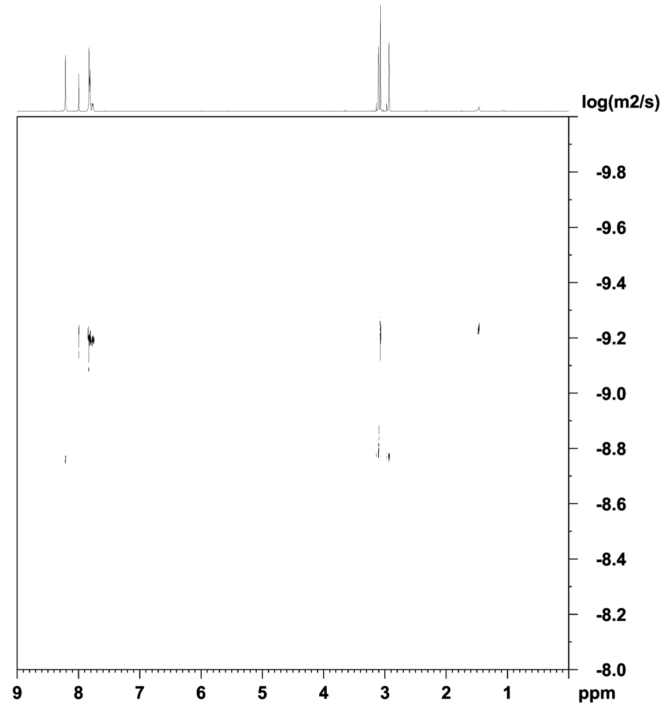
DOSY ^{1}H NMR spectrum of **5** at 25 °C (DMF-d_7)

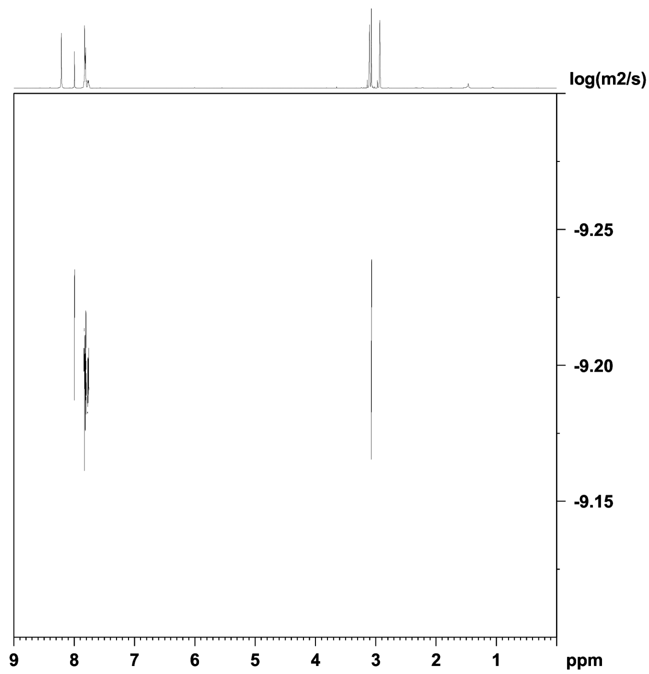




Spectrum of Bathocuproine (Bc)

DOSY ^{1}H NMR spectrum of **Bc** at 25 ºC (DMF-d_7)





Investigation of the silver species in solution

Based on the DOSY data along with the dynamic behavior observed by the 1D experiments, we hypothesized if, instead of the ligand, the solvent could play a crucial role in the observed equilibrium. Indeed, when the recrystallization of complex **5** was carried out in THF/hexane, we confirmed, by single crystal X-ray diffraction, the formation of $[(Bc)Ag(THF)]^{+}SbF_6^{-}$ (**6**) due to the displacement of a molecule of Bathocuproine by THF. Indeed, complex **6** can be independently prepared following the procedure in page S10. On the other hand, while **5** crystallizes in a traditional way with single isolated complexes; in **S1**, the external aromatic rings of the ligands are coordinated by hapticity with silver atoms of neighboring complexes forming a polymeric framework. One of the silver atoms shows η^3 bonding with distances of 2.25(2) Å, 2.59(2) Å and 2.59(3) Å and the other silver atom shows $\eta^2 + \eta^2$ bonding with distances of 2.51(2) Å and 2.60(2) Å to two symmetry equivalent aromatic rings.

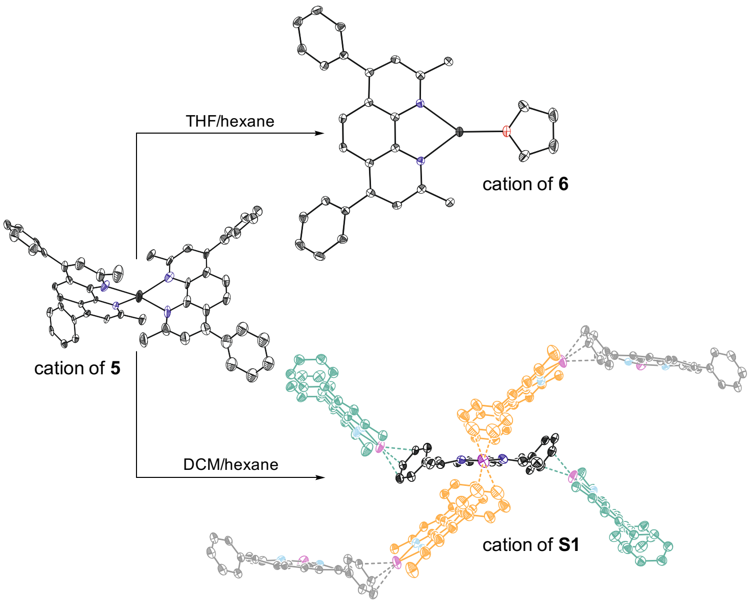


Figure S17. ORTEP structures for **5** and **6** are shown with thermal ellipsoids set at 50% of probability (H atoms and counter anion SbF_6^{-} have been omitted for clarity). ORTEP showing the interactions in the crystal packing for the structure of **S1** with thermal ellipsoids set at 50% of probability (H atoms, the counter anion SbF_6^{-} and solvent molecules have been omitted for clarity).

DFT calculations to investigate the nature of the cation of 4b, $(Cation)^{+}[Ag(CF_3)_2]^{-}$

A) Computational details

DFT calculations were performed with the ωB97-xD functional,[9] using the Gaussian09 package.[10] The basis set was SDD plus pseudopotential for silver,[11] and 6-31G(d)[12] for the remaining atoms. All geometry optimizations were carried out in solution without symmetry restrictions. Implicit solvent was modeled through the SMD method.[13] Calculations were carried out in two different solvents: THF (ε = 7.43) and DMF (ε = 37.22). Explicit solvent molecules were introduced when coordinating to the silver center. The number of required solvent molecules was decided through the application of a cluster continuum model, discussed in detail in the following section. Details on the application of this cluster continuum model are provided in the next section. All the energies presented are free energies in kcal/mol. All those reported in the main text and most of the Supporting Information are free energies at 25 ºC and 1 M, the only exception being those in the next section. The free energies provided by the standard Gaussian09 calculations at ideal gas concentrations were corrected by 1.895 kcal/mol in steps with change of molecularity. We are aware that 1 M is not the standard state for the solvent, but this is taken into account when computing equilibrium concentrations.

B) Election of optimal number of explicit solvent molecules

The computational prediction of the number of solvent molecules acting as ligand for a given solute is not trivial when implicit solvents are also used in the calculation. The main problem is the proper consideration of the entropic effects associated to the transfer of a solvent molecule from the bulk to the solute. A successful approach to overcome this problem has been the application of solvent clusters.[14] The basic idea is to consider a reaction of the type shown in eq. S2:

$$M(Solv)_m + (Solv)_n \rightarrow M(Solv)_{m+1} + (Solv)_{n-1} \qquad \text{(eq. S2)}$$

If the free energy associated to the process is negative, the solute *M* will adapt an extra solvent molecule in its coordination sphere.

The only practical problem with this approach is the need to find an appropriate size for the solvent cluster. The building of the cluster has been done by the subsequent addition of solvent molecules to a cluster of two molecules of THF or DMF. The election of the number of molecules that forms the cluster is associated to the minimal variation of the energy of the system when a solvent molecule is taken from the initial cluster. This process is represented in eq. S3:

$$(Solv)_n \rightarrow x\, Solv + (Solv)_{n-x} \qquad \text{(eq. S3)}$$

Where *n* is the number of molecules of the cluster and *x*, the number of molecules that is taken out from it.

The free energy difference for eq. S3 is reported in Table S4 for THF, and in Table S5 for DMF. In these cases, the uncorrected ΔG values for ideal gas concentration were used, as we are only interested in the trend. The trend in ΔG is asymptotic towards smaller values (minimum value) as the number of molecules in the cluster increases. The cluster must be large enough to produce a constant number upon addition of extra molecules. $(Solv)_7$ was taken as the optimal choice for the representation of the bulk of the solvent as reactant. We admit here that under ideal conditions the converged value for the addition of extra molecules should be 0.0 kcal/mol, and not 5.0 or 4.0 kcal/mol per solvent molecule, as shown in the Tables 4 and 5. This error is inherent to the problem of using together implicit/explicit models for the solvent, and the use of the cluster is precisely a solution to avoid it from entering the estimation of binding energy.

Table S4. Free energy values for the reaction in eq. S3 with THF as solvent

n(THF)	$\Delta G_{x=1}$ ($kcal \cdot mol^{-1}$)	$\Delta G_{x=2}$ ($kcal \cdot mol^{-1}$)
1	-	-
2	8.2	-
3	6.6	14.8
4	6.8	13.4
5	5.6	12.4
6	6.5	12.2
7	5.0	11.6
8	6.2	11.2

Table S5. Free energy values for the reaction in eq. S3 with DMF as solvent

n(DMF)	$\Delta G_{x=1}$ (kcal/mol)	$\Delta G_{x=2}$ (kcal/mol)
1	-	-
2	6.4	-
3	5.8	12.2
4	4.6	10.4
5	4.7	9.3
6	5.9	10.6
7	4.0	9.9
8	6.6	10.6

Thus, the expression in eq. S4 will be used to estimate the free energy associated to the presence of solvent molecules on silver.

$$A + (Solv)_7 \rightarrow A(Solv)_x + (Solv)_{7-x} \qquad \text{(eq. S4)}$$

For the calculation of equilibrium constants, the ΔG associated to eq. S4 is assumed to be the same that the one that corresponds to eq. S5. This is based on the assumption that the ΔG associated to eq. S3 should be zero.

$$A + x\,Solv \rightarrow B \qquad \text{(eq. S5)}$$

C) Election of the cation 4b-cat

We started by computing **4a** in THF, and to our surprise, computations show a significant stabilizing interaction between neighbouring molecules by π–π interactions, which prompts us to propose a dimeric structure for [(Bc)Ag(CF_3)]$_2$ (**4a'**), as shown in Figure S18a. The free energy of this dimer, which is stabilized by π–π interactions between the bathocuproine rings, is 15.8 kcal/mol below the separated monomers of **4a**.

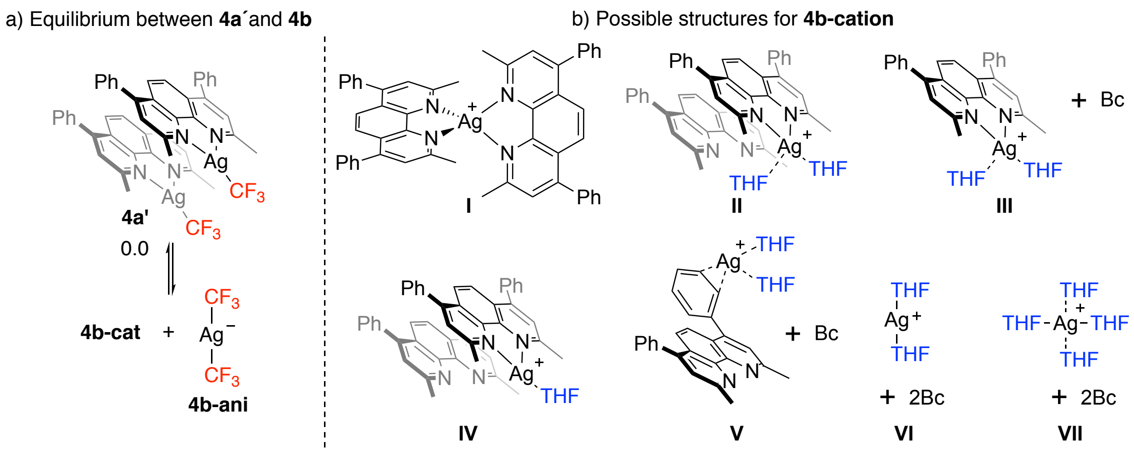


Figure S18. a) Equilibrium between **4a**´and **4b**. b) Different plausible forms for the **4b-cat** cation in THF

We next analyzed possible forms of the **4b-cat** cation. Different species were evaluated as candidates (Figure S18b). The free energy differences associate to their equilibrium with **4a'** are shown in Table S6. The solvent molecules were neglected from the equilibria in Table S6 for clarity. The most favorable cationic form is by far **II**.

Table S6. Free energy values for free ions equilibrium of **4a'** in THF.

Plausible equilibrium	ΔG (kcal/mol)
4a' ↔ I + 4b-ani	16.2
4a' ↔ II + 4b-ani	10.8
4a' ↔ III + 4b-ani	26.2
4a' ↔ IV + 4b-ani	18.3
4a' ↔ V + 4b-ani	49.1
4a' ↔ VI + 4b-ani	45.8
4a' ↔ VII + 4b-ani	36.8

D) Equilibrium concentrations from computed ΔG values

A ΔG value of 10.8 kcal/mol seems very large for species that are observed in equilibrium. This is however correct if we take into account the very different concentrations involved.

$$\Delta G = -RTln(K_{eq}) \qquad \text{(eq. S6)}$$

The equilibrium constant in THF for the equilibrium **4a' ↔ II + 4b-ani** has a value of:

$$K_{eq,THF} = 1.1 \cdot 10^{-8}\ \mathrm{M}^{-1}$$

The proportion in the equilibrium was calculated as follows:

4a'	+	2 THF	$\rightleftharpoons$	**4b-cat**	+	**4b-ani**
C_0		12.33		0		0
C_0 - x		12.33 - 2x		x		x

$$K_{eq,THF} = \frac{[\textbf{4b-cat}][\textbf{4b-ani}]}{[\textbf{4a'}][\textbf{THF}]^2} = \frac{x^2}{(C_0\text{-}x)[\textbf{THF}]^2} \qquad \text{(eq. S7)}$$

Taking into consideration that the experimental initial concentration of **4a** is $6.2 \cdot 10^{-3}$ M ($3.1 \cdot 10^{-3}$ M, for the calculated dimer **4a'**) and the concentration of THF is constant (12.33 M), the value for x is $7.12 \cdot 10^{-5}$ M, using eq. S7 and the proportion of **4a'** is 92%.

In the case of DMF, ΔG is 6.0 Kcal/mol and the equilibrium constant for the previous equilibrium takes a value of:

$$K_{eq,DMF} = 3.8 \cdot 10^{-5}\ \mathrm{M}^{-1}$$

The concentration of the solvent is 12.92 M and the value of x is $2.28 \cdot 10^{-3}$ M using eq. S7. The resulting proportion of **4a'** in DMF is thus 58%.

E) Free ions *vs* ion pair

Experimental evidences show a necessary contribution of ion pair interaction for the equilibrium of **4a'** in THF. Figure S19 shows a modified version of the leading equilibrium including the ion pair (**4b-ionpair**).

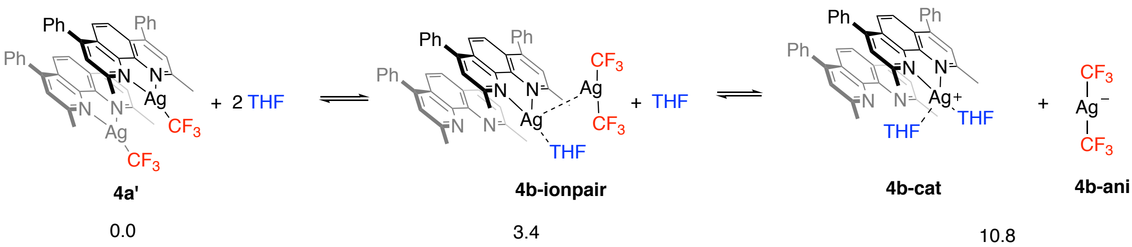


Figure S19. Modified version considering the contribution of ion pair.

Both simultaneous equilibria have been considered in order to calculate the final proportion of the ionic form. These results lead to a slightly more complicated expression:

4a'	+	2 THF	$\rightleftharpoons$	**4b-ionpair**	+	THF	$\rightleftharpoons$	**4b-cat**	+	**4b-ani**
C_0		12.33		0		0		0		0
C_0 - x		12.33 - 2x		x-y		12.33 - x - y		y		y

The constant for the two equilibria in THF are $3.14 \cdot 10^{-3}$ M^{-1} and $3.57 \cdot 10^{-6}$, respectively. The resulting values for x and y after solving the equations are, respectively, $7.0 \cdot 10^{-5}$ M and $1.8 \cdot 10^{-4}$ M. The final proportion of the ionic form in this equilibrium is 8% (75% of ion pair and 25% of free ions).
We repeated the same treatment for the solution in DMF and there is no contribution of ion pairs.

F) Cartesian coordinates (Å) and potential energies (u.a.) of the optimized structures

In THF

Cluster-1_THF

Energy(POTENTIAL) = -232.38199289

Atom	X	Y	Z
C	4.0257	14.6461	2.5859
O	4.8922	13.6416	2.0610
C	6.0788	14.2441	1.5566
C	6.1480	15.6323	2.1858
C	4.6630	15.9975	2.2539
H	3.0291	14.5268	2.1450
H	3.9353	14.5054	3.6723
H	6.9297	13.6047	1.8152
H	6.0253	14.3163	0.4591
H	6.5757	15.5724	3.1931
H	6.7444	16.3331	1.5952
H	4.4338	16.7618	3.0013
H	4.3166	16.3562	1.2779

Cluster-2_THF

Energy(POTENTIAL) = -464.76504499

Atom	X	Y	Z
C	9.2546	15.6497	1.0847
O	9.6328	14.2783	1.1273
C	10.8637	14.1397	1.8358
C	11.1983	15.5182	2.4090
C	10.5167	16.4453	1.4003
H	8.8363	15.8676	0.0966
H	8.4764	15.8431	1.8389
H	10.7494	13.3733	2.6113
H	11.6404	13.8016	1.1354
H	10.7455	15.6428	3.3995
H	12.2748	15.6845	2.5003
H	10.3022	17.4415	1.7965
H	11.1328	16.5515	0.5000
C	6.4531	16.8861	6.5033
O	6.3336	16.1994	5.2595
C	6.4385	17.1273	4.1833
C	6.9609	18.4285	4.7868
C	6.3409	18.3755	6.1851
H	5.6692	16.5305	7.1813
H	7.4279	16.6541	6.9578
H	7.1028	16.7087	3.4191
H	5.4481	17.2755	3.7276
H	8.0549	18.4061	4.8552
H	6.6679	19.3092	4.2092
H	6.8538	19.0034	6.9183
H	5.2882	18.6784	6.1437

Cluster-3_THF

Energy(POTENTIAL) = -697.15831252

Atom	X	Y	Z
C	10.6621	14.3049	1.4107
O	10.9308	13.2095	2.2783
C	11.0247	13.6728	3.6249
C	10.6208	15.1485	3.6119
C	11.0237	15.5626	2.1942
H	11.2490	14.1772	0.4947
H	9.5954	14.3108	1.1356
H	10.3741	13.0604	4.2601
H	12.0595	13.5448	3.9741
H	9.5374	15.2482	3.7420
H	11.1216	15.7246	4.3953
H	10.4995	16.4504	1.8294
H	12.1025	15.7492	2.1380
C	4.4470	20.7710	4.2021
O	4.2797	19.5752	3.4388
C	4.8223	19.7560	2.1327
C	5.7109	20.9934	2.2100
C	4.9506	21.8406	3.2332
H	3.4904	21.0297	4.6691
H	5.1796	20.5858	5.0006
H	5.3633	18.8456	1.8523
H	4.0052	19.9043	1.4110
H	6.7014	20.7286	2.5982
H	5.8367	21.4840	1.2411
H	5.5725	22.5919	3.7272
H	4.1084	22.3508	2.7520
C	7.2348	16.6915	4.8736
O	7.2252	15.8110	3.7479
C	7.4023	16.5604	2.5498
C	7.9948	17.8979	2.9761
C	7.2898	18.1165	4.3173
H	6.3397	16.5064	5.4780
H	8.1175	16.4660	5.4881
H	8.0486	15.9858	1.8776
H	6.4296	16.7024	2.0537
H	9.0774	17.8054	3.1226
H	7.8099	18.6921	2.2474
H	7.8220	18.8026	4.9821
H	6.2770	18.5012	4.1538

Cluster-4_THF

Energy(POTENTIAL) = -929.55084031

Atom	X	Y	Z
C	4.9798	16.0770	1.5505
O	5.0470	14.6668	1.4565
C	6.4036	14.3029	1.1952
C	7.1383	15.5804	0.7365
C	5.9943	16.5818	0.5313
H	3.9485	16.3826	1.3493
H	5.2492	16.4131	2.5671
H	6.8510	13.8746	2.1019

H	6.3925	13.5279	0.4207
H	7.8171	15.9439	1.5151
H	7.7253	15.4165	-0.1715
H	6.2974	17.6194	0.6993
H	5.5744	16.5009	-0.4773
C	8.5972	14.5354	4.1303
O	7.9589	13.2667	4.2668
C	8.8279	12.2348	3.8007
C	10.1862	12.8888	3.5474
C	9.7744	14.3181	3.1870
H	7.8644	15.2539	3.7520
H	8.9421	14.8841	5.1159
H	8.8685	11.4391	4.5532
H	8.4150	11.8088	2.8751
H	10.7895	12.8865	4.4626
H	10.7522	12.3830	2.7603
H	10.5626	15.0606	3.3272
H	9.4385	14.3664	2.1446
C	4.3369	19.4176	2.6802
O	4.7981	20.7441	2.9363
C	4.7998	20.9928	4.3404
C	4.6891	19.6296	5.0163
C	3.8274	18.8626	4.0102
H	3.5642	19.4512	1.9042
H	5.1768	18.8208	2.3006
H	5.7179	21.5318	4.5968
H	3.9420	21.6307	4.6011
H	5.6777	19.1650	5.1061
H	4.2445	19.6912	6.0131
H	3.9399	17.7771	4.0795
H	2.7691	19.1083	4.1508
C	7.9640	18.1212	3.5908
O	9.0644	17.5381	2.9041
C	9.3458	18.3885	1.8050
C	9.2214	19.8010	2.3723
C	8.0680	19.6505	3.3856
H	7.0202	17.7346	3.1764
H	8.0291	17.8126	4.6378
H	10.3421	18.1384	1.4318
H	8.6162	18.2255	0.9948
H	10.1505	20.0779	2.8803
H	9.0166	20.5472	1.5999
H	8.2867	20.1689	4.3233
H	7.1315	20.0567	2.9929

Cluster-5_THF

Energy(POTENTIAL) = -1161.94560096

Atom	X	Y	Z
C	4.8385	16.1607	1.6348
O	4.8262	14.9790	2.4365
C	5.8127	14.0944	1.9273
C	6.9475	15.0010	1.4652
C	6.1698	16.1761	0.8567
H	3.9753	16.1545	0.9545
H	4.7355	17.0182	2.3082
H	6.0880	13.4031	2.7288
H	5.4082	13.5098	1.0842
H	7.5313	15.3264	2.3330
H	7.6177	14.5127	0.7511
H	6.6769	17.1362	0.9717
H	5.9835	16.0212	-0.2101
C	9.1843	13.0237	3.3189
O	9.7215	12.0781	4.2394
C	10.8096	12.6708	4.9470
C	10.8974	14.1276	4.4831
C	10.2906	14.0439	3.0813
H	8.8739	12.4860	2.4167
H	8.3053	13.5188	3.7562
H	10.6332	12.5800	6.0256
H	11.7297	12.1191	4.7066
H	10.2672	14.7674	5.1099
H	11.9208	14.5128	4.5009
H	9.9075	14.9998	2.7164
H	11.0225	13.6557	2.3625
C	4.7795	20.0114	1.9315
O	6.0033	19.4350	1.4727
C	7.0735	20.3623	1.6376
C	6.5692	21.4076	2.6259
C	5.0852	21.4740	2.2545
H	4.0165	19.8918	1.1542
H	4.4476	19.4681	2.8268
H	7.9539	19.8121	1.9852
H	7.3158	20.8233	0.6686
H	6.6907	21.0493	3.6547
H	7.0864	22.3655	2.5266
H	4.4512	21.8642	3.0549
H	4.9451	22.1014	1.3669
C	6.8309	16.5516	4.8073
O	8.1611	16.1589	4.4499
C	8.9351	17.3100	4.1268
C	8.1912	18.4932	4.7357
C	6.7388	18.0532	4.5321
H	6.1185	15.9613	4.2216
H	6.6764	16.3328	5.8729
H	9.9451	17.1707	4.5258
H	9.0078	17.4172	3.0331
H	8.4226	18.5811	5.8036
H	8.4352	19.4412	4.2482
H	6.0310	18.5559	5.1973
H	6.4381	18.2398	3.4948
C	4.7585	18.4082	-1.5680
O	5.3782	17.3070	-2.2303
C	6.7538	17.6021	-2.4693
C	7.0542	18.9135	-1.7432
C	5.6880	19.6007	-1.7650
H	3.7621	18.5525	-1.9993
H	4.6513	18.1847	-0.4976
H	7.3672	16.7675	-2.1104
H	6.9130	17.7020	-3.5525
H	7.3472	18.7174	-0.7069
H	7.8460	19.4887	-2.2311
H	5.5715	20.3504	-0.9783
H	5.5091	20.0751	-2.7370

Cluster-6_THF

Energy(POTENTIAL) = -1394.34265603

Atom	X	Y	Z
C	5.2289	15.9907	1.4015
O	4.8393	14.7696	0.7900
C	5.1685	13.7493	1.7194

C	6.4646	14.1970	2.4259
C	6.5816	15.6866	2.0433
H	5.2598	16.7580	0.6264
H	4.4905	16.2876	2.1659
H	4.3511	13.6311	2.4495
H	5.2683	12.8112	1.1658
H	6.3935	14.0718	3.5100
H	7.3394	13.6375	2.0840
H	6.7993	16.3283	2.8989
H	7.3764	15.8280	1.3062
C	9.8391	14.9004	3.1771
O	9.8392	13.9330	2.1243
C	10.1249	14.5709	0.8855
C	10.8435	15.8681	1.2428
C	10.1177	16.2609	2.5313
H	8.8759	14.8693	3.6985
H	10.6261	14.6297	3.8943
H	10.7292	13.8888	0.2787
H	9.1900	14.7766	0.3415
H	11.9036	15.6721	1.4401
H	10.7709	16.6242	0.4558
H	10.6990	16.9163	3.1823
H	9.1800	16.7731	2.2964
C	5.4394	20.1095	2.1655
O	6.2039	18.9074	2.1467
C	7.5936	19.2073	2.2981
C	7.6960	20.7222	2.4949
C	6.4179	21.2249	1.8179
H	4.6196	20.0017	1.4489
H	5.0086	20.2603	3.1670
H	7.9997	18.6503	3.1478
H	8.1156	18.8807	1.3883
H	7.6850	20.9665	3.5629
H	8.6087	21.1372	2.0598
H	6.0882	22.2025	2.1802
H	6.5560	21.2838	0.7318
C	5.6993	16.3073	5.4729
O	7.0256	15.7834	5.4747
C	7.9688	16.8451	5.6136
C	7.1737	18.0872	6.0082
C	5.8305	17.8219	5.3215
H	5.1383	15.8426	4.6535
H	5.2059	16.0417	6.4195
H	8.7149	16.5526	6.3608
H	8.4848	17.0080	4.6586
H	7.0461	18.1361	7.0959
H	7.6660	19.0030	5.6701
H	4.9947	18.3579	5.7807
H	5.8808	18.0958	4.2616
C	6.4682	18.7023	-1.2816
O	5.9259	17.4439	-1.6731
C	6.9561	16.4539	-1.6598
C	8.2374	17.1522	-1.1905
C	7.9639	18.6113	-1.5627
H	5.9605	19.4866	-1.8529
H	6.2838	18.8662	-0.2110
H	6.6518	15.6291	-1.0049
H	7.0702	16.0576	-2.6781
H	8.3485	17.0618	-0.1039
H	9.1342	16.7372	-1.6592
H	8.5493	19.3264	-0.9768
H	8.1655	18.7831	-2.6262
C	10.8921	19.7051	3.4756
O	10.0857	19.1121	4.4931
C	10.9132	18.5736	5.5215
C	12.2891	19.2038	5.3270
C	12.3408	19.3424	3.8032
H	10.5677	19.3273	2.4989
H	10.7418	20.7932	3.4917
H	10.4573	18.8043	6.4896
H	10.9677	17.4794	5.4183
H	12.3291	20.1902	5.8028
H	13.0943	18.5878	5.7361
H	13.0493	20.0992	3.4566
H	12.6094	18.3841	3.3436

Cluster-7_THF

Energy(POTENTIAL) = -1626.73348300

Atom	X	Y	Z
C	5.4594	16.0711	0.3448
O	6.5194	15.4192	-0.3418
C	7.4820	15.0795	0.6384
C	7.5458	16.2921	1.5663
C	6.0951	16.8138	1.5425
H	4.9699	16.7353	-0.3718
H	4.7282	15.3262	0.6953
H	7.1697	14.1782	1.1931
H	8.4222	14.8596	0.1256
H	7.9010	16.0326	2.5670
H	8.2300	17.0398	1.1530
H	5.5629	16.5873	2.4712
H	6.0589	17.8972	1.4024
C	10.5250	13.7213	2.1914
O	10.3836	12.4428	2.8015
C	11.1806	12.3869	3.9829
C	11.8131	13.7706	4.1598
C	11.8383	14.2892	2.7196
H	10.5078	13.5833	1.1055
H	9.6872	14.3719	2.4819
H	10.5495	12.1022	4.8338
H	11.9468	11.6090	3.8544
H	11.1621	14.4082	4.7665
H	12.8006	13.7214	4.6270
H	11.8854	15.3797	2.6517
H	12.6876	13.8682	2.1685
C	2.9629	20.5214	1.5040
O	3.9468	19.6282	2.0256
C	5.1103	20.3590	2.4018
C	4.7114	21.8323	2.4134
C	3.6618	21.8641	1.2994
H	2.5579	20.0989	0.5784
H	2.1411	20.6124	2.2288
H	5.4605	19.9903	3.3723
H	5.9014	20.1814	1.6604
H	4.2575	22.1005	3.3739
H	5.5600	22.4984	2.2339
H	2.9714	22.7087	1.3706
H	4.1499	21.8992	0.3184
C	8.1209	16.3373	5.3574
O	9.2263	15.9395	4.5514
C	10.0054	17.0859	4.1946
C	9.3907	18.2801	4.9266
C	7.9380	17.8294	5.1039

H	7.2530	15.7337	5.0726
H	8.3431	16.1436	6.4178
H	11.0501	16.9078	4.4748
H	9.9544	17.2302	3.1088
H	9.8622	18.4216	5.9058
H	9.5007	19.2035	4.3524
H	7.4189	18.3363	5.9220
H	7.3695	17.9848	4.1793
C	5.0928	19.6097	-1.2945
O	5.4713	18.4777	-2.0643
C	6.8759	18.3591	-1.9153
C	7.3981	19.7910	-2.0342
C	6.2647	20.6147	-1.3855
H	4.1574	19.9941	-1.7113
H	4.9085	19.3117	-0.2518
H	7.1234	17.9260	-0.9344
H	7.2404	17.6788	-2.6885
H	8.3635	19.9249	-1.5368
H	7.5184	20.0593	-3.0883
H	6.5450	20.9735	-0.3908
H	6.0053	21.4882	-1.9898
C	8.5027	19.7446	1.6820
O	9.8321	19.2380	1.6674
C	10.7503	20.2754	1.3082
C	9.8998	21.4726	0.8852
C	8.6325	21.2639	1.7174
H	7.9722	19.4140	0.7754
H	7.9818	19.3280	2.5486
H	11.3654	20.5176	2.1861
H	11.4054	19.9027	0.5144
H	10.3975	22.4269	1.0761
H	9.6630	21.4166	-0.1838
H	8.7861	21.6093	2.7463
H	7.7553	21.7743	1.3105
C	12.2031	17.1855	0.2430
O	12.3582	18.1556	-0.7958
C	11.3342	17.9719	-1.7655
C	10.1673	17.3485	-1.0107
C	10.9034	16.4193	-0.0420
H	13.0790	16.5248	0.2591
H	12.1567	17.7179	1.2003
H	11.1082	18.9476	-2.2069
H	11.6850	17.3031	-2.5678
H	9.6328	18.1197	-0.4480
H	9.4641	16.8248	-1.6640
H	10.3380	16.2264	0.8723
H	11.1177	15.4582	-0.5221

Cluster-8_THF

Energy(POTENTIAL) = -2091.52314217

Atom	X	Y	Z
C	5.4773	16.2687	0.6567
O	6.0012	15.0578	0.1238
C	7.2653	14.7945	0.7349
C	7.6397	16.0398	1.5555
C	6.7032	17.1046	0.9870
H	4.8321	16.7233	-0.0986
H	4.8867	16.0671	1.5666
H	7.1970	13.8959	1.3622
H	7.9914	14.5960	-0.0639
H	7.4383	15.8826	2.6196
H	8.6957	16.2995	1.4568
H	6.5088	17.9345	1.6697
H	7.1128	17.5222	0.0617
C	10.0861	14.1661	3.1327
O	9.9654	12.9909	3.9168
C	10.6018	13.3049	5.1446
C	11.8291	14.1687	4.7865
C	11.5278	14.6396	3.3455
H	9.8474	13.9083	2.0967
H	9.3716	14.9246	3.4862
H	9.9118	13.8699	5.7912
H	10.8514	12.3649	5.6441
H	11.9364	15.0150	5.4705
H	12.7531	13.5846	4.8283
H	11.6361	15.7215	3.2335
H	12.1957	14.1537	2.6273
C	4.6930	19.7048	2.6891
O	5.9106	20.2617	2.1900
C	5.6851	21.5975	1.7355
C	4.1726	21.8071	1.7454
C	3.7424	20.8810	2.8852
H	4.2933	18.9901	1.9547
H	4.9115	19.1636	3.6153
H	6.1835	22.2954	2.4207
H	6.1288	21.7131	0.7410
H	3.8993	22.8536	1.9041
H	3.7322	21.4726	0.7995
H	3.9221	21.3593	3.8550
H	2.6918	20.5840	2.8329
C	7.2051	17.7547	4.8320
O	8.3346	16.9053	4.9635
C	9.4230	17.5980	4.3733
C	9.2533	19.0564	4.8041
C	7.7211	19.2059	4.9333
H	6.7214	17.5886	3.8586
H	6.4929	17.4847	5.6169
H	10.3493	17.1381	4.7263
H	9.3818	17.5187	3.2755
H	9.7445	19.2256	5.7677
H	9.6898	19.7422	4.0736
H	7.4451	19.6615	5.8885
H	7.2977	19.8186	4.1312
C	5.2464	19.6159	-1.2375
O	4.9748	18.3465	-1.8205
C	6.1339	17.8837	-2.5169
C	7.1895	18.9945	-2.4191
C	6.3362	20.2282	-2.1090
H	4.3133	20.1883	-1.2305
H	5.5934	19.4998	-0.1995
H	6.4703	16.9382	-2.0735
H	5.8508	17.6890	-3.5591
H	7.8841	18.8004	-1.5932
H	7.7763	19.0898	-3.3366
H	6.8883	21.0250	-1.6032
H	5.8998	20.6365	-3.0276
C	12.7542	18.4535	3.6679
O	12.9060	17.4598	4.6840
C	14.1536	16.7891	4.5235
C	14.9781	17.6427	3.5639
C	13.8823	18.2198	2.6642
H	11.7638	18.3601	3.2156
H	12.8311	19.4490	4.1310

H	14.6152	16.6695	5.5098
H	13.9833	15.7888	4.1007
H	15.4910	18.4459	4.1060
H	15.7258	17.0576	3.0214
H	14.1824	19.1387	2.1523
H	13.5735	17.4889	1.9080
C	8.6442	22.7557	3.5497
O	9.9916	23.1065	3.8124
C	10.3054	22.6400	5.1209
C	8.9779	22.5633	5.9072
C	7.9155	22.9794	4.8725
H	8.2912	23.3898	2.7317
H	8.5661	21.7021	3.2362
H	10.7846	21.6527	5.0613
H	11.0243	23.3425	5.5529
H	8.8035	21.5456	6.2666
H	8.9795	23.2262	6.7764
H	6.9938	22.3949	4.9482
H	7.6629	24.0386	4.9836
C	9.1305	19.7087	1.1193
O	10.4439	19.4486	1.5972
C	11.1216	20.6925	1.6865
C	10.6658	21.4711	0.4560
C	9.2051	21.0094	0.2898
H	8.8246	18.8411	0.5296
H	8.4288	19.8110	1.9574
H	10.8461	21.2276	2.6069
H	12.1955	20.4882	1.7062
H	10.7599	22.5516	0.5915
H	11.2644	21.1789	-0.4135
H	8.5049	21.7551	0.6770
H	8.9589	20.8347	-0.7609
C	11.0998	16.3804	0.2272
O	12.4373	16.6956	-0.1246
C	12.3786	17.9750	-0.7417
C	11.0390	18.0318	-1.5096
C	10.2788	16.7903	-0.9976
H	11.0532	15.3129	0.4574
H	10.7970	16.9586	1.1135
H	12.4095	18.7582	0.0268
H	13.2582	18.0724	-1.3837
H	10.5040	18.9574	-1.2801
H	11.1880	17.9909	-2.5920
H	9.2322	16.9971	-0.7552
H	10.2997	15.9897	-1.7436

4b-ionpair_THF

Energy(POTENTIAL) = -3425.62699103

Atom	X	Y	Z
Ag	7.3677	10.6345	0.6186
C	6.3955	11.8521	-3.2654
C	6.5874	13.1736	-3.7054
H	7.0842	13.3501	-4.6543
C	6.1238	14.2401	-2.9578
C	5.4544	13.9504	-1.7346
C	5.2662	12.5897	-1.4013
N	5.7445	11.5743	-2.1478
C	5.0054	14.9546	-0.8102
H	5.2594	15.9919	-0.9952
C	4.2904	14.6312	0.2952
H	3.9864	15.4134	0.9814
C	4.5128	12.2408	-0.1985
C	3.9578	13.2667	0.5990
C	3.1307	12.8753	1.6913
C	3.0036	11.5227	1.9466
H	2.3665	11.1789	2.7554
C	3.6651	10.5757	1.1451
N	4.3839	10.9294	0.0918
C	6.9154	10.6876	-4.0625
H	6.0913	10.0272	-4.3540
H	7.6129	10.0948	-3.4623
H	7.4333	11.0178	-4.9674
C	6.3273	15.6181	-3.4780
C	7.5698	15.9802	-4.0144
H	8.3886	15.2676	-3.9927
C	7.7716	17.2439	-4.5574
H	8.7473	17.5096	-4.9531
C	6.7315	18.1701	-4.5751
H	6.8885	19.1594	-4.9949
C	5.4881	17.8200	-4.0536
H	4.6679	18.5318	-4.0762
C	5.2853	16.5534	-3.5120
H	4.3028	16.2820	-3.1371
C	2.3747	13.8371	2.5363
C	1.6618	14.9042	1.9732
H	1.6704	15.0536	0.8977
C	0.9102	15.7574	2.7765
H	0.3619	16.5766	2.3205
C	0.8499	15.5546	4.1533
H	0.2643	16.2217	4.7790
C	1.5427	14.4888	4.7225
H	1.5110	14.3270	5.7959
C	2.2972	13.6396	3.9209
H	2.8466	12.8216	4.3762
C	3.5594	9.1052	1.4395
H	2.9397	8.6093	0.6831
H	3.1110	8.9214	2.4199
H	4.5539	8.6506	1.4045
C	8.9107	13.0687	-0.9816
C	9.2249	14.3961	-1.3287
H	9.7923	14.5781	-2.2359
C	8.7871	15.4508	-0.5603
C	8.0612	15.1484	0.6275
C	7.7706	13.7949	0.8999
N	8.1770	12.7886	0.0857
C	7.6608	16.1566	1.5619
H	7.9531	17.1848	1.3849
C	6.9597	15.8430	2.6769
H	6.6963	16.6215	3.3831
C	7.0192	13.4579	2.1017
C	6.5968	14.4889	2.9658
C	5.8614	14.1241	4.1306
C	5.6643	12.7839	4.3745
H	5.1195	12.4619	5.2567
C	6.1309	11.8127	3.4673
N	6.7659	12.1520	2.3579
C	9.4232	11.9458	-1.8299
H	10.4663	11.7303	-1.5675
H	9.3984	12.2103	-2.8918
H	8.8442	11.0338	-1.6776
C	9.0716	16.8419	-0.9961
C	10.3656	17.1971	-1.3925
H	11.1667	16.4665	-1.3221

C	10.6344	18.4806	-1.8590
H	11.6457	18.7435	-2.1553
C	9.6129	19.4244	-1.9391
H	9.8224	20.4255	-2.3045
C	8.3200	19.0774	-1.5523
H	7.5148	19.8020	-1.6274
C	8.0501	17.7953	-1.0859
H	7.0330	17.5254	-0.8173
C	5.3062	15.1321	5.0699
C	4.4909	16.1727	4.6089
H	4.2671	16.2540	3.5489
C	3.9355	17.0822	5.5029
H	3.2946	17.8762	5.1312
C	4.1841	16.9629	6.8687
H	3.7509	17.6738	7.5663
C	4.9902	15.9274	7.3368
H	5.1902	15.8285	8.3997
C	5.5459	15.0159	6.4434
H	6.1833	14.2157	6.8098
C	5.9020	10.3591	3.7581
H	4.8547	10.1751	4.0191
H	6.5159	10.0447	4.6099
H	6.1666	9.7408	2.8967
C	6.1665	8.0081	-0.9143
O	6.7294	8.4625	0.3362
C	7.2834	7.3576	1.0719
C	6.6594	6.1209	0.4455
C	6.5653	6.5420	-1.0243
H	5.0816	8.1423	-0.8589
H	6.5574	8.6349	-1.7161
H	8.3729	7.3582	0.9513
H	7.0420	7.5040	2.1282
H	7.2711	5.2288	0.6014
H	5.6619	5.9405	0.8622
H	7.5456	6.4536	-1.5023
H	5.8387	5.9599	-1.5967
Ag	10.1737	9.5034	0.7437
C	10.2282	10.3969	2.6525
F	10.0659	11.7674	2.7152
F	11.4220	10.1972	3.3230
F	9.2852	9.9234	3.5527
C	10.1774	8.5105	-1.1244
F	9.0482	8.6291	-1.9234
F	10.3401	7.1390	-1.0341
F	11.1956	8.8917	-1.9790

4a_THF

Energy(POTENTIAL) = -1596.59228271

Atom	X	Y	Z
Ag	4.1202	11.9448	1.6184
C	2.8308	13.1728	0.4906
C	3.8288	8.6664	1.7095
C	4.1724	7.3323	1.9924
H	3.5524	6.5319	1.6015
C	5.3012	7.0342	2.7290
C	6.0881	8.1158	3.2163
C	5.6810	9.4219	2.8756
N	4.5788	9.6745	2.1363
C	7.2320	7.9412	4.0653
H	7.5001	6.9417	4.3882
C	7.9620	9.0016	4.4885
H	8.8086	8.8431	5.1468
C	6.4650	10.5610	3.3296
C	7.6198	10.3421	4.1073
C	8.3649	11.4843	4.5144
C	7.8881	12.7305	4.1622
H	8.4321	13.6228	4.4549
C	6.7167	12.8627	3.3946
N	6.0383	11.7974	2.9857
C	2.6082	8.9976	0.9006
H	1.9225	9.6195	1.4861
H	2.0804	8.0925	0.5893
H	2.8849	9.5677	0.0071
C	5.6523	5.6117	2.9783
C	4.6994	4.7444	3.5242
H	3.7224	5.1296	3.8030
C	5.0018	3.4007	3.7257
H	4.2559	2.7395	4.1567
C	6.2559	2.9057	3.3746
H	6.4899	1.8566	3.5293
C	7.2073	3.7609	2.8220
H	8.1834	3.3794	2.5369
C	6.9098	5.1061	2.6261
H	7.6510	5.7649	2.1825
C	9.6227	11.3786	5.2986
C	10.7044	10.6252	4.8270
H	10.6209	10.0963	3.8817
C	11.8915	10.5701	5.5509
H	12.7268	9.9900	5.1700
C	12.0101	11.2596	6.7562
H	12.9367	11.2129	7.3207
C	10.9381	12.0116	7.2316
H	11.0232	12.5489	8.1716
C	9.7523	12.0749	6.5051
H	8.9150	12.6577	6.8792
C	6.2119	14.2153	2.9837
H	6.2866	14.3329	1.8967
H	6.7856	15.0155	3.4584
H	5.1569	14.3306	3.2528
F	1.5245	12.7261	0.3862
F	3.2082	13.3439	-0.8297
F	2.6775	14.4723	0.9420

4b-cat-II_THF

Energy(POTENTIAL) = -2835.78194900

Atom	X	Y	Z
Ag	7.2070	10.5629	0.3214
C	6.2786	11.9133	-3.4507
C	6.4569	13.2419	-3.8729
H	6.9157	13.4351	-4.8375
C	6.0270	14.2955	-3.0877
C	5.4042	13.9841	-1.8449
C	5.2292	12.6181	-1.5286
N	5.6761	11.6150	-2.3116
C	4.9892	14.9710	-0.8867
H	5.2341	16.0118	-1.0629
C	4.3155	14.6278	0.2385
H	4.0320	15.3978	0.9468
C	4.5268	12.2484	-0.3016
C	3.9975	13.2578	0.5323

C	3.2160	12.8456	1.6502
C	3.0964	11.4880	1.8851
H	2.4882	11.1302	2.7099
C	3.7341	10.5575	1.0477
N	4.4217	10.9320	-0.0200
C	6.7526	10.7633	-4.2969
H	5.9003	10.1631	-4.6341
H	7.4075	10.1074	-3.7140
H	7.3000	11.1098	-5.1780
C	6.2188	15.6812	-3.5906
C	7.4409	16.0435	-4.1725
H	8.2569	15.3274	-4.1925
C	7.6275	17.3131	-4.7065
H	8.5870	17.5788	-5.1396
C	6.5928	18.2449	-4.6692
H	6.7379	19.2383	-5.0832
C	5.3706	17.8957	-4.0993
H	4.5549	18.6125	-4.0785
C	5.1826	16.6231	-3.5664
H	4.2151	16.3524	-3.1541
C	2.5033	13.7922	2.5478
C	1.7598	14.8666	2.0412
H	1.7069	15.0319	0.9693
C	1.0554	15.7072	2.8985
H	0.4808	16.5320	2.4873
C	1.0754	15.4849	4.2736
H	0.5275	16.1434	4.9410
C	1.7998	14.4121	4.7870
H	1.8323	14.2370	5.8583
C	2.5059	13.5740	3.9315
H	3.0829	12.7511	4.3421
C	3.6521	9.0812	1.3202
H	3.1275	8.5714	0.5045
H	3.1254	8.8712	2.2551
H	4.6588	8.6563	1.3833
C	8.8806	12.9691	-1.2157
C	9.1909	14.2941	-1.5780
H	9.7157	14.4727	-2.5112
C	8.8001	15.3523	-0.7867
C	8.1241	15.0545	0.4326
C	7.8232	13.7044	0.7078
N	8.1857	12.6954	-0.1227
C	7.7855	16.0582	1.3965
H	8.0900	17.0830	1.2206
C	7.1278	15.7436	2.5381
H	6.9118	16.5184	3.2644
C	7.1188	13.3657	1.9362
C	6.7515	14.3930	2.8290
C	6.0634	14.0247	4.0220
C	5.8726	12.6830	4.2654
H	5.3663	12.3565	5.1687
C	6.2891	11.7161	3.3293
N	6.8645	12.0586	2.1889
C	9.3488	11.8322	-2.0762
H	10.4246	11.6741	-1.9328
H	9.1883	12.0484	-3.1367
H	8.8276	10.9058	-1.8176
C	9.0829	16.7433	-1.2242
C	10.3576	17.0829	-1.6906
H	11.1488	16.3384	-1.6800
C	10.6223	18.3697	-2.1509
H	11.6187	18.6204	-2.5030
C	9.6157	19.3325	-2.1538
H	9.8220	20.3363	-2.5135
C	8.3413	19.0012	-1.6983
H	7.5465	19.7407	-1.7143
C	8.0755	17.7162	-1.2390
H	7.0704	17.4598	-0.9178
C	5.5510	15.0296	4.9876
C	4.7436	16.0897	4.5585
H	4.4959	16.1870	3.5052
C	4.2242	16.9970	5.4759
H	3.5886	17.8060	5.1287
C	4.5017	16.8562	6.8340
H	4.0966	17.5653	7.5500
C	5.2998	15.8010	7.2708
H	5.5210	15.6849	8.3277
C	5.8194	14.8918	6.3539
H	6.4499	14.0760	6.6971
C	6.0645	10.2612	3.6203
H	5.0001	10.0586	3.7831
H	6.5977	9.9697	4.5327
H	6.4213	9.6368	2.7969
C	6.0567	8.0285	-1.4161
O	6.9795	8.3623	-0.3614
C	7.0986	7.2671	0.5680
C	6.0561	6.2408	0.1356
C	5.9361	6.5129	-1.3668
H	5.1015	8.5271	-1.2213
H	6.4701	8.4149	-2.3502
H	8.1165	6.8688	0.4939
H	6.9445	7.6504	1.5801
H	6.3672	5.2190	0.3663
H	5.0982	6.4306	0.6320
H	6.7651	6.0435	-1.9080
H	4.9951	6.1590	-1.7951
C	9.9637	10.5939	2.3146
O	9.3006	9.5956	1.5245
C	10.2456	8.9394	0.6706
C	11.4866	9.8233	0.6700
C	11.4595	10.3836	2.0942
H	9.6462	11.5842	1.9662
H	9.6539	10.4731	3.3571
H	10.4686	7.9452	1.0812
H	9.7893	8.8154	-0.3157
H	12.3971	9.2650	0.4372
H	11.3774	10.6326	-0.0612
H	11.8544	9.6451	2.8008
H	12.0272	11.3107	2.2083

4b-ani_THF

Energy(POTENTIAL) = -822.20451629

Atom	X	Y	Z
Ag	4.2847	12.0277	1.4133
C	2.8188	13.0833	0.3290
F	1.9483	12.3006	-0.4077
F	3.3121	13.9721	-0.6097
F	1.9684	13.8679	1.0865
C	5.7548	10.9719	2.4913
F	6.1732	9.7865	1.9139
F	5.3883	10.5865	3.7683
F	6.9405	11.6540	2.6985

4b-cat-I_THF

Energy(POTENTIAL) = -2370.97792954

Atom	X	Y	Z
Ag	3.9704	11.7605	1.8472
C	3.7522	8.4994	2.0405
C	4.1383	7.1874	2.3656
H	3.4996	6.3582	2.0790
C	5.3318	6.9471	3.0161
C	6.1426	8.0621	3.3704
C	5.6825	9.3453	3.0089
N	4.5150	9.5384	2.3538
C	7.3703	7.9393	4.1031
H	7.6923	6.9574	4.4307
C	8.1185	9.0271	4.4086
H	9.0353	8.9073	4.9746
C	6.4773	10.5162	3.3554
C	7.7077	10.3464	4.0218
C	8.4624	11.5150	4.3242
C	7.9239	12.7420	3.9954
H	8.4717	13.6531	4.2145
C	6.6811	12.8266	3.3423
N	5.9943	11.7365	3.0259
C	2.4675	8.7770	1.3146
H	1.8266	9.4348	1.9130
H	1.9201	7.8545	1.1048
H	2.6683	9.2873	0.3655
C	5.7214	5.5469	3.3293
C	4.8646	4.7413	4.0865
H	3.9378	5.1584	4.4711
C	5.2019	3.4192	4.3625
H	4.5341	2.8060	4.9604
C	6.3929	2.8856	3.8749
H	6.6532	1.8527	4.0864
C	7.2467	3.6796	3.1116
H	8.1714	3.2658	2.7203
C	6.9162	5.0044	2.8420
H	7.5794	5.6169	2.2373
C	9.7998	11.4480	4.9691
C	10.8452	10.7346	4.3705
H	10.6722	10.2095	3.4349
C	12.1059	10.7104	4.9590
H	12.9123	10.1616	4.4816
C	12.3342	11.3915	6.1534
H	13.3170	11.3672	6.6146
C	11.2985	12.1040	6.7538
H	11.4697	12.6339	7.6862
C	10.0387	12.1379	6.1620
H	9.2300	12.6898	6.6331
C	6.1062	14.1533	2.9378
H	6.2178	14.2972	1.8562
H	6.6115	14.9802	3.4436
H	5.0361	14.1973	3.1674
C	4.0581	12.7640	-1.2571
C	3.6363	13.4274	-2.4219
H	4.2350	13.3502	-3.3236
C	2.4615	14.1527	-2.4338
C	1.7030	14.2219	-1.2312
C	2.1947	13.5271	-0.1069
N	3.3458	12.8177	-0.1392
C	0.5037	14.9995	-1.1028
H	0.1640	15.5842	-1.9499
C	-0.1923	15.0332	0.0594
H	-1.0864	15.6418	0.1325
C	1.4553	13.5772	1.1475
C	0.2471	14.3009	1.2126
C	-0.4518	14.3079	2.4529
C	0.1193	13.6547	3.5268
H	-0.3860	13.6435	4.4870
C	1.3399	12.9724	3.3830
N	1.9714	12.9305	2.2173
C	5.3278	11.9630	-1.2326
H	5.9995	12.3367	-0.4512
H	5.8488	12.0119	-2.1921
H	5.1117	10.9122	-1.0066
C	2.0483	14.8438	-3.6834
C	2.9396	15.7251	-4.3054
H	3.9060	15.9187	-3.8482
C	2.5879	16.3643	-5.4905
H	3.2851	17.0533	-5.9578
C	1.3456	16.1222	-6.0723
H	1.0717	16.6198	-6.9979
C	0.4562	15.2380	-5.4644
H	-0.5098	15.0393	-5.9189
C	0.8027	14.6030	-4.2753
H	0.1099	13.9064	-3.8113
C	-1.7618	14.9883	2.6234
C	-2.8528	14.6561	1.8116
H	-2.7374	13.9043	1.0354
C	-4.0864	15.2699	2.0061
H	-4.9274	14.9983	1.3750
C	-4.2427	16.2253	3.0088
H	-5.2046	16.7073	3.1564
C	-3.1616	16.5596	3.8215
H	-3.2760	17.3055	4.6025
C	-1.9288	15.9405	3.6346
H	-1.0852	16.2068	4.2656
C	1.9683	12.2434	4.5356
H	1.9849	11.1647	4.3400
H	1.4222	12.4167	5.4664
H	3.0058	12.5683	4.6721

4b-cat-VII_THF

Energy(POTENTIAL) = -1076.47003132

Atom	X	Y	Z
Ag	4.0687	12.0483	1.8379
C	1.0914	10.6968	2.4630
O	1.8274	11.4541	1.4847
C	0.9298	12.2469	0.6816
C	-0.4409	12.1061	1.3351
C	-0.3512	10.7195	1.9793
H	1.5287	9.6965	2.5110
H	1.1978	11.1814	3.4418
H	1.2983	13.2761	0.6626
H	0.9407	11.8447	-0.3377
H	-0.5788	12.8741	2.1040
H	-1.2514	12.1928	0.6077
H	-1.0640	10.5768	2.7949
H	-0.5146	9.9371	1.2304
C	5.5523	11.7967	4.8323
O	5.3099	12.7086	3.7428
C	6.4329	13.5935	3.5705

C	7.2487	13.4608	4.8489
C	7.0127	11.9940	5.2213
H	4.8726	12.0566	5.6519
H	5.3248	10.7824	4.4923
H	7.0058	13.2762	2.6897
H	6.0431	14.5993	3.3951
H	8.3030	13.7001	4.6912
H	6.8515	14.1233	5.6254
H	7.6608	11.3413	4.6252
H	7.1880	11.7834	6.2788
C	4.5632	8.8010	2.2380
O	5.2195	9.9819	1.7412
C	6.6423	9.8916	1.9511
C	6.8508	8.6758	2.8459
C	5.6741	7.7804	2.4456
H	4.0603	9.0424	3.1834
H	3.8137	8.4983	1.5026
H	7.1251	9.7676	0.9751
H	6.9854	10.8283	2.3989
H	7.8246	8.2076	2.6843
H	6.7723	8.9581	3.9022
H	5.8920	7.2574	1.5083
H	5.4165	7.0399	3.2064
C	3.5734	15.2369	1.2281
O	4.0314	14.0361	0.5805
C	3.7490	14.0873	-0.8336
C	2.8977	15.3356	-1.0394
C	3.3660	16.2413	0.1038
H	2.6345	15.0241	1.7562
H	4.3304	15.5342	1.9580
H	4.7044	14.1500	-1.3661
H	3.2419	13.1615	-1.1201
H	3.0467	15.7761	-2.0280
H	1.8344	15.0989	-0.9220
H	4.3130	16.7279	-0.1529
H	2.6380	17.0118	0.3682

4b-cat-VI_THF

Energy(POTENTIAL) = -611.66122892

Atom	X	Y	Z
Ag	4.0527	10.8880	2.4941
C	1.3287	10.3270	0.8824
O	2.0900	11.2869	1.6623
C	1.5195	12.6153	1.5458
C	0.1505	12.3922	0.9230
C	0.3965	11.1731	0.0290
H	2.0324	9.7234	0.3052
H	0.7837	9.6852	1.5819
H	1.4902	13.0535	2.5455
H	2.1717	13.2147	0.9017
H	-0.5880	12.1579	1.6964
H	-0.1895	13.2693	0.3681
H	-0.5202	10.6357	-0.2236
H	0.8944	11.4721	-0.8992
C	6.3158	10.3120	4.6865
O	6.0319	10.4670	3.2734
C	7.2601	10.6272	2.5141
C	8.3580	10.7503	3.5621
C	7.7894	9.9473	4.7363
H	6.1102	11.2637	5.1884
H	5.6469	9.5411	5.0744
H	7.3785	9.7371	1.8892
H	7.1566	11.5098	1.8791
H	9.3093	10.3577	3.1962
H	8.4994	11.7978	3.8475
H	7.9220	8.8735	4.5686
H	8.2429	10.2117	5.6940

Bc-Ligand_THF

Energy(POTENTIAL) = -1112.00383035

Atom	X	Y	Z
C	4.0505	12.7403	-1.2071
C	3.6559	13.4234	-2.3779
H	4.2683	13.3502	-3.2723
C	2.4895	14.1555	-2.3970
C	1.7187	14.2153	-1.1993
C	2.1989	13.5056	-0.0760
N	3.3416	12.7809	-0.0939
C	0.5201	14.9939	-1.0799
H	0.1885	15.5841	-1.9272
C	-0.1886	15.0211	0.0761
H	-1.0843	15.6291	0.1427
C	1.4509	13.5570	1.1751
C	0.2416	14.2851	1.2295
C	-0.4688	14.2938	2.4656
C	0.0955	13.6415	3.5394
H	-0.4134	13.6268	4.4991
C	1.3257	12.9638	3.3943
N	1.9708	12.9102	2.2437
C	5.3170	11.9284	-1.2050
H	6.1848	12.5607	-1.4272
H	5.2805	11.1463	-1.9721
H	5.4625	11.4598	-0.2289
C	2.0903	14.8623	-3.6441
C	2.9810	15.7603	-4.2425
H	3.9392	15.9560	-3.7689
C	2.6420	16.4118	-5.4249
H	3.3407	17.1125	-5.8727
C	1.4103	16.1680	-6.0283
H	1.1456	16.6755	-6.9514
C	0.5200	15.2687	-5.4441
H	-0.4384	15.0683	-5.9142
C	0.8558	14.6203	-4.2588
H	0.1624	13.9123	-3.8133
C	-1.7809	14.9757	2.6258
C	-2.8698	14.6398	1.8123
H	-2.7504	13.8845	1.0402
C	-4.1049	15.2540	1.9975
H	-4.9426	14.9787	1.3633
C	-4.2675	16.2139	2.9950
H	-5.2307	16.6955	3.1364
C	-3.1896	16.5527	3.8100
H	-3.3075	17.3019	4.5876
C	-1.9551	15.9344	3.6297
H	-1.1141	16.2049	4.2625
C	1.9424	12.2672	4.5763
H	1.2578	11.5194	4.9929
H	2.1657	12.9843	5.3750
H	2.8692	11.7719	4.2783

4b-cat-V_THF

Energy(POTENTIAL) = -1723.68709056

Atom	X	Y	Z
C	4.3569	13.9468	-1.7539
C	3.8821	14.8718	-2.7077
H	4.4919	15.1109	-3.5743
C	2.6392	15.4473	-2.5561
C	1.8818	15.1227	-1.3976
C	2.4322	14.1707	-0.5083
N	3.6418	13.5982	-0.6998
C	0.6306	15.7472	-1.0801
H	0.2503	16.5333	-1.7239
C	-0.0616	15.3988	0.0324
H	-0.9912	15.9063	0.2656
C	1.6775	13.7847	0.6794
C	0.4232	14.3860	0.9258
C	-0.2861	13.9789	2.0940
C	0.3095	13.0494	2.9174
H	-0.1993	12.7091	3.8149
C	1.5720	12.5088	2.5894
N	2.2296	12.8616	1.4998
C	5.7007	13.2973	-1.9400
H	6.4526	14.0279	-2.2555
H	5.6514	12.5212	-2.7142
H	6.0244	12.8274	-1.0083
C	2.1324	16.3555	-3.6242
C	2.8929	17.4567	-4.0370
H	3.8309	17.6724	-3.5344
C	2.4491	18.2779	-5.0697
H	3.0457	19.1358	-5.3645
C	1.2508	18.0049	-5.7275
H	0.9125	18.6454	-6.5357
C	0.4754	16.9166	-5.3296
H	-0.4772	16.7146	-5.8100
C	0.9002	16.0966	-4.2697
H	0.2391	15.3202	-3.8880
C	-1.6252	14.5216	2.4482
C	-2.7039	14.4273	1.5607
H	-2.5623	13.9612	0.5895
C	-3.9589	14.9085	1.9218
H	-4.7875	14.8243	1.2246
C	-4.1520	15.4926	3.1723
H	-5.1307	15.8714	3.4520
C	-3.0853	15.5866	4.0633
H	-3.2278	16.0419	5.0390
C	-1.8304	15.1014	3.7050
H	-0.9986	15.1808	4.3999
C	2.2077	11.4913	3.4961
H	1.5263	10.6540	3.6848
H	2.4492	11.9385	4.4676
H	3.1277	11.1087	3.0484
Ag	2.0476	14.5789	-5.7168
C	1.7808	11.3317	-6.3380
O	1.1271	12.6043	-6.5339
C	0.3559	12.5927	-7.7535
C	0.2401	11.1245	-8.1359
C	1.5750	10.5636	-7.6371
H	2.8328	11.5157	-6.1035
H	1.3056	10.8344	-5.4855
H	-0.6017	13.0778	-7.5489
H	0.8937	13.1679	-8.5175
H	-0.5956	10.6560	-7.6054
H	0.0906	10.9892	-9.2095
H	1.5554	9.4835	-7.4754
H	2.3745	10.7943	-8.3502
C	5.1091	13.2559	-5.7103
O	4.1437	13.9902	-6.4974
C	4.2605	13.6382	-7.8915
C	5.6153	12.9598	-8.0168
C	5.7315	12.2455	-6.6668
H	5.8488	13.9701	-5.3325
H	4.5901	12.7970	-4.8642
H	3.4437	12.9550	-8.1549
H	4.1621	14.5574	-8.4739
H	5.6556	12.2768	-8.8685
H	6.4081	13.7071	-8.1270
H	5.1499	11.3169	-6.6763
H	6.7617	12.0060	-6.3935

4b-cat-IV_THF

Energy(POTENTIAL) = -2603.37997052

Atom	X	Y	Z
Ag	7.0996	10.6427	0.3881
C	6.3289	11.9291	-3.3619
C	6.5012	13.2569	-3.7896
H	6.9795	13.4485	-4.7450
C	6.0434	14.3115	-3.0216
C	5.3939	14.0022	-1.7919
C	5.2250	12.6371	-1.4717
N	5.7044	11.6327	-2.2337
C	4.9478	14.9895	-0.8480
H	5.1891	16.0313	-1.0229
C	4.2487	14.6461	0.2617
H	3.9427	15.4170	0.9595
C	4.4954	12.2677	-0.2608
C	3.9331	13.2748	0.5530
C	3.1231	12.8581	1.6490
C	3.0062	11.4998	1.8830
H	2.3747	11.1393	2.6887
C	3.6817	10.5722	1.0729
N	4.4012	10.9511	0.0272
C	6.8381	10.7788	-4.1863
H	6.0057	10.1431	-4.5076
H	7.5177	10.1573	-3.5934
H	7.3716	11.1258	-5.0756
C	6.2347	15.6961	-3.5272
C	7.4682	16.0677	-4.0782
H	8.2917	15.3601	-4.0727
C	7.6562	17.3369	-4.6129
H	8.6242	17.6105	-5.0216
C	6.6119	18.2586	-4.6064
H	6.7581	19.2517	-5.0208
C	5.3785	17.8996	-4.0677
H	4.5556	18.6086	-4.0711
C	5.1888	16.6275	-3.5345
H	4.2133	16.3487	-3.1471
C	2.3807	13.8008	2.5258
C	1.6487	14.8735	1.9995
H	1.6250	15.0397	0.9268
C	0.9181	15.7110	2.8378
H	0.3531	16.5346	2.4113

C	0.9004	15.4873	4.2126
H	0.3319	16.1434	4.8651
C	1.6128	14.4156	4.7452
H	1.6144	14.2387	5.8166
C	2.3446	13.5804	3.9088
H	2.9102	12.7571	4.3340
C	3.6083	9.0962	1.3486
H	3.1213	8.5777	0.5152
H	3.0486	8.8828	2.2633
H	4.6166	8.6827	1.4530
C	8.8579	12.9931	-1.0811
C	9.1671	14.3193	-1.4381
H	9.7093	14.4990	-2.3610
C	8.7552	15.3766	-0.6566
C	8.0559	15.0768	0.5492
C	7.7606	13.7255	0.8233
N	8.1448	12.7169	0.0010
C	7.6857	16.0818	1.4996
H	7.9853	17.1082	1.3256
C	7.0015	15.7669	2.6253
H	6.7586	16.5430	3.3414
C	7.0299	13.3862	2.0356
C	6.6289	14.4146	2.9120
C	5.9075	14.0476	4.0855
C	5.7122	12.7063	4.3267
H	5.1788	12.3813	5.2148
C	6.1611	11.7371	3.4086
N	6.7762	12.0778	2.2874
C	9.3505	11.8599	-1.9314
H	10.4146	11.6824	-1.7317
H	9.2479	12.0910	-2.9958
H	8.8048	10.9374	-1.7126
C	9.0417	16.7681	-1.0901
C	10.3269	17.1114	-1.5239
H	11.1204	16.3702	-1.4897
C	10.5986	18.3979	-1.9805
H	11.6033	18.6517	-2.3057
C	9.5884	19.3564	-2.0139
H	9.8001	20.3599	-2.3711
C	8.3036	19.0212	-1.5914
H	7.5065	19.7573	-1.6310
C	8.0309	17.7367	-1.1346
H	7.0184	17.4780	-0.8396
C	5.3658	15.0531	5.0343
C	4.5599	16.1052	4.5831
H	4.3338	16.1968	3.5245
C	4.0152	17.0126	5.4856
H	3.3811	17.8156	5.1220
C	4.2659	16.8801	6.8498
H	3.8413	17.5896	7.5540
C	5.0626	15.8330	7.3081
H	5.2637	15.7238	8.3697
C	5.6071	14.9231	6.4064
H	6.2366	14.1136	6.7659
C	5.9233	10.2843	3.6962
H	4.8587	10.0923	3.8682
H	6.4624	9.9833	4.6021
H	6.2634	9.6598	2.8656
C	6.1706	8.0664	-1.2816
O	7.0212	8.4410	-0.1755
C	7.1429	7.3480	0.7606
C	6.1516	6.2909	0.2884
C	6.0948	6.5488	-1.2202
H	5.1922	8.5379	-1.1451
H	6.6278	8.4565	-2.1933
H	8.1765	6.9869	0.7227
H	6.9360	7.7245	1.7662
H	6.4816	5.2804	0.5409
H	5.1673	6.4573	0.7392
H	6.9608	6.1000	-1.7187
H	5.1848	6.1642	-1.6868

4b-cat-III_THF

Energy(POTENTIAL) = -1723.72355651

Atom	X	Y	Z
Ag	7.2520	10.4625	0.6434
C	8.5920	12.8137	-1.2184
C	8.9889	14.1104	-1.5918
H	9.5074	14.2550	-2.5342
C	8.6882	15.1941	-0.7926
C	8.0077	14.9555	0.4359
C	7.6394	13.6274	0.7329
N	7.9235	12.5950	-0.0950
C	7.7328	15.9889	1.3918
H	8.0759	16.9970	1.1896
C	7.0811	15.7209	2.5493
H	6.9107	16.5164	3.2654
C	6.9451	13.3378	1.9812
C	6.6423	14.3925	2.8674
C	5.9558	14.0673	4.0721
C	5.6749	12.7390	4.3233
H	5.1534	12.4567	5.2322
C	6.0316	11.7442	3.3972
N	6.6340	12.0506	2.2562
C	8.9293	11.6264	-2.0723
H	9.8173	11.1225	-1.6709
H	9.1449	11.9200	-3.1031
H	8.1060	10.9041	-2.0721
C	9.0782	16.5590	-1.2333
C	10.4096	16.8324	-1.5642
H	11.1597	16.0531	-1.4597
C	10.7783	18.0990	-2.0091
H	11.8169	18.3023	-2.2522
C	9.8192	19.1009	-2.1394
H	10.1071	20.0880	-2.4890
C	8.4891	18.8328	-1.8214
H	7.7353	19.6073	-1.9284
C	8.1194	17.5701	-1.3681
H	7.0796	17.3621	-1.1317
C	5.5403	15.0971	5.0594
C	4.7473	16.1859	4.6774
H	4.4437	16.2941	3.6399
C	4.3294	17.1176	5.6228
H	3.7074	17.9532	5.3158
C	4.7022	16.9758	6.9581
H	4.3769	17.7047	7.6943
C	5.4908	15.8947	7.3459
H	5.7852	15.7789	8.3848
C	5.9046	14.9580	6.4033
H	6.5255	14.1196	6.7069
C	5.7385	10.2945	3.6551
H	5.1000	9.8880	2.8622
H	5.2348	10.1514	4.6144

H	6.6706	9.7178	3.6628
C	5.9040	8.1206	-1.2862
O	6.6708	8.4136	-0.1011
C	7.1478	7.2005	0.5150
C	6.3807	6.0792	-0.1730
C	6.1736	6.6513	-1.5793
H	4.8462	8.3077	-1.0682
H	6.2309	8.7984	-2.0789
H	8.2270	7.1228	0.3407
H	6.9638	7.2738	1.5898
H	6.9364	5.1385	-0.1681
H	5.4156	5.9174	0.3191
H	7.0869	6.5410	-2.1738
H	5.3472	6.1814	-2.1175
C	10.0961	10.7969	2.2705
O	9.4742	9.7518	1.5031
C	10.4276	9.1688	0.6001
C	11.6426	10.0899	0.6247
C	11.5952	10.6293	2.0569
H	9.7475	11.7679	1.8952
H	9.7797	10.6884	3.3115
H	10.6805	8.1636	0.9599
H	9.9642	9.0809	-0.3874
H	12.5687	9.5595	0.3894
H	11.5190	10.9087	-0.0936
H	12.0035	9.8924	2.7573
H	12.1374	11.5696	2.1844

4a'_THF

Energy(POTENTIAL) = -3193.24057977

Atom	X	Y	Z
Ag	3.9436	12.4878	2.9465
C	2.7949	13.4503	1.4571
N	5.8579	12.4066	4.3144
F	2.9313	14.8223	1.3427
F	1.4260	13.2791	1.5427
F	3.0773	13.0079	0.1677
N	4.4114	10.2386	3.6078
C	6.5635	13.4938	4.5997
C	6.2925	11.1993	4.7411
C	3.6895	9.2055	3.1970
C	5.5095	10.0307	4.3624
C	6.0500	14.8135	4.1043
C	7.7767	13.4083	5.3027
C	7.4655	11.0350	5.5054
C	2.4844	9.4896	2.3481
C	4.0532	7.8897	3.5263
C	5.9221	8.7471	4.7734
H	4.9821	14.9176	4.3160
H	6.1763	14.8812	3.0171
H	6.5872	15.6474	4.5642
C	8.2598	12.1936	5.7507
H	8.3537	14.3143	5.4557
C	7.7734	9.7280	6.0154
H	1.8588	10.2588	2.8115
H	2.7943	9.8710	1.3683
H	1.8851	8.5881	2.1954
C	5.1656	7.6336	4.3061
H	3.4629	7.0671	3.1358
C	7.0397	8.6421	5.6683
C	9.5887	12.1490	6.4144
H	8.5938	9.6149	6.7146
C	5.5211	6.2214	4.5988
H	7.2870	7.6744	6.0881
C	9.9465	13.1429	7.3342
C	10.5377	11.1742	6.0780
C	4.5221	5.3211	4.9910
C	6.8260	5.7450	4.4235
C	11.2074	13.1511	7.9192
H	9.2248	13.9059	7.6074
C	11.8000	11.1828	6.6648
H	10.2998	10.4220	5.3322
C	4.8206	3.9822	5.2152
H	3.5064	5.6777	5.1348
C	7.1241	4.4040	4.6490
H	7.6061	6.4192	4.0822
C	12.1373	12.1678	7.5902
H	11.4575	13.9180	8.6459
H	12.5247	10.4235	6.3868
C	6.1242	3.5201	5.0477
H	4.0371	3.3025	5.5358
H	8.1396	4.0482	4.5016
H	13.1202	12.1705	8.0516
H	6.3587	2.4750	5.2269
Ag	3.3018	12.4503	6.3668
C	2.0483	13.9586	5.5698
F	2.6349	14.9085	4.7454
F	0.9550	13.5420	4.8345
F	1.4723	14.7402	6.5627
N	3.6969	10.2566	7.0717
N	5.2132	12.3783	7.8329
H	7.5425	14.2293	9.3687
C	5.8944	13.4459	8.2213
C	6.9926	13.3344	9.0949
C	7.3944	12.1039	9.5700
C	6.6322	10.9622	9.1928
C	5.5507	11.1603	8.3117
C	4.7416	10.0234	7.9017
C	5.0560	8.7376	8.3867
C	6.1236	8.5912	9.3329
C	6.8774	9.6503	9.7145
C	4.2587	7.6462	7.9383
C	3.1871	7.9296	7.1165
C	2.9165	9.2475	6.7059
H	6.3059	7.6193	9.7758
H	9.9044	13.4258	13.2465
H	7.6580	9.5161	10.4545
H	4.7155	15.2196	8.4000
H	4.9874	14.7056	6.7339
H	6.3002	15.4864	7.6581
C	5.4585	14.7901	7.7161
H	9.5899	10.5268	9.2378
H	11.5995	10.4355	10.6659
H	11.7693	11.8864	12.6769
C	8.6990	12.8324	11.5704
C	9.8362	12.7859	12.3717
C	10.8806	11.9201	12.0535
C	10.7832	11.1012	10.9303
C	9.6455	11.1437	10.1306
C	8.5906	12.0088	10.4446
C	1.7181	9.5475	5.8548
H	7.8830	13.5033	11.8246
C	4.5466	6.2365	8.3074

H	0.8769	9.8427	6.4947
H	1.9205	10.3784	5.1742
H	1.4108	8.6721	5.2755
H	2.5501	7.1288	6.7563
C	3.5080	5.4009	8.7337
C	5.8337	5.7004	8.1744
C	3.7524	4.0628	9.0280
H	2.5067	5.8065	8.8498
C	6.0768	4.3636	8.4694
H	6.6454	6.3244	7.8136
C	5.0372	3.5405	8.8975
H	2.9373	3.4286	9.3641
H	7.0774	3.9603	8.3472
H	5.2269	2.4955	9.1241

In DMF

Cluster-1_DMF

Energy(POTENTIAL) = -248.43822384

Atom	X	Y	Z
C	-0.5176	1.2255	-0.9154
O	-0.3924	1.7808	-1.9997
N	0.4379	1.1252	0.0350
H	-1.4605	0.7354	-0.6151
C	0.1933	0.4736	1.3049
H	0.2926	1.1899	2.1298
H	-0.8166	0.0558	1.3237
H	0.9125	-0.3387	1.4622
C	1.7450	1.7172	-0.1593
H	1.7837	2.1646	-1.1530
H	1.9316	2.4909	0.5953
H	2.5258	0.9521	-0.0744

Cluster-2_DMF

Energy(POTENTIAL) = -496.88575123

Atom	X	Y	Z
C	-0.6477	1.2909	-0.8238
O	-0.6063	1.8176	-1.9294
N	0.3990	1.1534	0.0210
H	-1.5785	0.8711	-0.4093
C	0.2573	0.5365	1.3220
H	0.4818	1.2567	2.1183
H	-0.7650	0.1735	1.4551
H	0.9450	-0.3120	1.4188
C	1.7157	1.6295	-0.3427
H	1.6668	2.0614	-1.3427
H	2.0583	2.3925	0.3668
H	2.4371	0.8032	-0.3361
C	-0.4753	-2.2133	-0.4079
O	-1.5402	-1.8688	-0.9072
N	0.7453	-2.0496	-0.9610
H	-0.4251	-2.7054	0.5791
C	1.9465	-2.5323	-0.3138
H	2.4331	-3.3011	-0.9265
H	2.6568	-1.7112	-0.1611
H	1.6987	-2.9662	0.6582
C	0.8978	-1.4375	-2.2645
H	-0.0531	-0.9974	-2.5638
H	1.6616	-0.6539	-2.2217
H	1.2057	-2.1833	-3.0082

Cluster-3_DMF

Energy(POTENTIAL) = -745.33280386

Atom	X	Y	Z
C	-1.5733	1.7673	0.3444
O	-2.5497	2.5052	0.2337
N	-0.2863	2.1466	0.1939
H	-1.6739	0.6952	0.5829
C	0.8041	1.2047	0.3417
H	1.5269	1.5773	1.0767
H	0.4181	0.2451	0.6908
H	1.3239	1.0564	-0.6130
C	0.0629	3.5182	-0.1127
H	-0.8481	4.1163	-0.1434
H	0.7331	3.9168	0.6579
H	0.5724	3.5801	-1.0816
C	-0.3649	-2.1320	-0.2152
O	-1.3610	-1.8668	0.4512
N	-0.0881	-1.6455	-1.4421
H	0.4137	-2.8220	0.1526
C	1.1611	-1.9325	-2.1151
H	0.9759	-2.4020	-3.0880
H	1.7266	-1.0067	-2.2781
H	1.7668	-2.6091	-1.5067
C	-0.9908	-0.7204	-2.0953
H	-1.9256	-0.6844	-1.5359
H	-0.5502	0.2831	-2.1390
H	-1.1951	-1.0575	-3.1174
C	-3.5403	1.2058	-2.9451
O	-4.2562	0.2909	-3.3352
N	-2.4990	1.7352	-3.6270
H	-3.6863	1.6888	-1.9637
C	-1.7111	2.8233	-3.0876
H	-1.7448	3.6904	-3.7585
H	-2.1035	3.1132	-2.1102
H	-0.6633	2.5181	-2.9714
C	-2.1093	1.2129	-4.9186
H	-2.7767	0.3917	-5.1816
H	-2.1747	1.9944	-5.6851
H	-1.0760	0.8462	-4.8847

Cluster-4_DMF

Energy(POTENTIAL) = -993.78543896

Atom	X	Y	Z
C	-0.2718	2.3321	0.6030
O	-1.3912	2.8442	0.6334
N	0.7115	2.6649	-0.2561
H	0.0222	1.5296	1.2965
C	2.0024	2.0022	-0.2276
H	2.7912	2.7124	0.0468
H	1.9801	1.1837	0.4959
H	2.2345	1.5879	-1.2155
C	0.5158	3.6973	-1.2553
H	-0.3105	4.3428	-0.9558

H	1.4277	4.2966	-1.3398
H	0.2930	3.2584	-2.2359
C	0.1410	-1.7054	1.0697
O	0.7449	-0.7300	1.5091
N	-0.1460	-1.9339	-0.2259
H	-0.2328	-2.5010	1.7363
C	-0.8033	-3.1512	-0.6569
H	-1.7201	-2.9143	-1.2091
H	-0.1449	-3.7370	-1.3091
H	-1.0665	-3.7594	0.2122
C	0.2595	-0.9919	-1.2519
H	0.3683	-0.0039	-0.8049
H	1.2143	-1.2874	-1.7050
H	-0.5103	-0.9419	-2.0287
C	-2.3668	1.1834	-2.5641
O	-2.3777	0.0631	-3.0732
N	-3.2649	2.1571	-2.7985
H	-1.5858	1.4874	-1.8471
C	-3.1747	3.4526	-2.1514
H	-4.1456	3.7056	-1.7137
H	-2.4386	3.4139	-1.3443
H	-2.8944	4.2300	-2.8729
C	-4.3975	1.9287	-3.6711
H	-4.2911	0.9500	-4.1399
H	-5.3258	1.9589	-3.0888
H	-4.4385	2.7013	-4.4474
C	-4.6044	1.4747	0.0263
O	-5.6316	2.0060	-0.3866
N	-4.2530	0.1874	-0.1747
H	-3.8551	2.0267	0.6180
C	-3.0021	-0.3480	0.3221
H	-2.3985	-0.7109	-0.5145
H	-2.4457	0.4339	0.8446
H	-3.1838	-1.1821	1.0111
C	-5.0577	-0.6852	-1.0027
H	-5.9821	-0.1692	-1.2642
H	-4.5098	-0.9422	-1.9174
H	-5.2971	-1.6079	-0.4612

Cluster-5_DMF

Energy(POTENTIAL) = -1242.23522534

Atom	X	Y	Z
C	-0.6176	2.6941	0.3450
O	-1.6055	2.9016	1.0494
N	0.0844	3.6417	-0.3087
H	-0.2229	1.6817	0.1669
C	1.2631	3.3076	-1.0833
H	2.1636	3.7271	-0.6182
H	1.3651	2.2220	-1.1525
H	1.1745	3.7172	-2.0960
C	-0.2624	5.0432	-0.2005
H	-1.1872	5.1357	0.3695
H	0.5352	5.5967	0.3102
H	-0.4018	5.4762	-1.1976
C	0.4986	-1.0724	-0.6733
O	0.4092	-0.0216	-1.3105
N	1.1965	-2.1547	-1.0581
H	-0.0042	-1.2069	0.2975
C	1.2485	-3.3579	-0.2513
H	0.8358	-4.2078	-0.8072
H	2.2856	-3.5876	0.0184
H	0.6681	-3.2197	0.6639
C	1.9285	-2.1691	-2.3087
H	1.8198	-1.1996	-2.7947
H	2.9900	-2.3650	-2.1194
H	1.5395	-2.9538	-2.9674
C	-3.8425	1.9772	-3.5470
O	-3.6722	1.0589	-4.3473
N	-2.8679	2.6869	-2.9492
H	-4.8528	2.3069	-3.2523
C	-3.1711	3.7354	-1.9940
H	-2.7335	4.6847	-2.3242
H	-4.2537	3.8596	-1.9124
H	-2.7744	3.4902	-1.0037
C	-1.4703	2.3948	-3.2080
H	-1.3869	1.8547	-4.1523
H	-0.9138	3.3347	-3.2819
H	-1.0329	1.7838	-2.4095
C	-4.5468	1.3008	-0.0178
O	-5.6668	1.7512	0.1989
N	-4.2671	0.2480	-0.8188
H	-3.6405	1.7278	0.4456
C	-2.9033	-0.1744	-1.0617
H	-2.6598	-0.0766	-2.1240
H	-2.2152	0.4488	-0.4874
H	-2.7640	-1.2222	-0.7677
C	-5.3200	-0.4521	-1.5249
H	-6.2825	-0.0836	-1.1676
H	-5.2402	-0.2794	-2.6044
H	-5.2444	-1.5297	-1.3456
C	-3.4848	-2.3832	-3.7800
O	-4.2744	-3.2371	-3.3897
N	-2.1431	-2.4275	-3.6252
H	-3.8146	-1.4722	-4.3066
C	-1.2854	-1.3633	-4.1083
H	-0.5829	-1.7458	-4.8594
H	-1.8989	-0.5745	-4.5517
H	-0.7114	-0.9287	-3.2809
C	-1.5155	-3.5224	-2.9176
H	-2.2806	-4.2524	-2.6515
H	-0.7587	-4.0024	-3.5492
H	-1.0305	-3.1556	-2.0056

Cluster-6_DMF

Energy(POTENTIAL) = -1490.68909612

Atom	X	Y	Z
C	-0.9860	2.1450	-0.6163
O	-2.0853	2.5638	-0.2518
N	-0.3438	2.5103	-1.7426
H	-0.4180	1.4092	-0.0250
C	0.9507	1.9529	-2.0850
H	1.7056	2.7464	-2.1391
H	1.2484	1.2255	-1.3257
H	0.9019	1.4534	-3.0598
C	-0.9080	3.4830	-2.6556
H	-1.8291	3.8797	-2.2280
H	-0.1983	4.3033	-2.8128
H	-1.1239	3.0182	-3.6244
C	1.2564	-1.5241	0.6354
O	1.1151	-0.3156	0.4552

N	1.8922	-2.3734	-0.1926
H	0.8501	-2.0242	1.5295
C	2.0675	-3.7728	0.1438
H	1.7004	-4.4062	-0.6713
H	3.1279	-3.9968	0.3094
H	1.5098	-4.0118	1.0524
C	2.5188	-1.9143	-1.4164
H	2.3214	-0.8506	-1.5487
H	3.6018	-2.0784	-1.3706
H	2.1175	-2.4671	-2.2729
C	-3.6330	1.6806	-3.2661
O	-3.2682	0.9461	-4.1841
N	-4.4117	2.7697	-3.4004
H	-3.3270	1.5082	-2.2236
C	-4.7687	3.5910	-2.2599
H	-5.8505	3.5517	-2.0914
H	-4.2408	3.2359	-1.3716
H	-4.4787	4.6324	-2.4434
C	-4.9346	3.1605	-4.6926
H	-4.6543	2.4055	-5.4276
H	-6.0260	3.2373	-4.6386
H	-4.5223	4.1312	-4.9942
C	-3.9497	-0.2950	-0.1174
O	-5.0858	-0.1045	-0.5494
N	-3.4750	-1.4750	0.3260
H	-3.2125	0.5214	-0.0461
C	-2.1230	-1.6088	0.8254
H	-1.5961	-2.3986	0.2790
H	-1.5781	-0.6712	0.6945
H	-2.1277	-1.8691	1.8912
C	-4.3027	-2.6631	0.3321
H	-5.3085	-2.3900	0.0117
H	-3.8992	-3.4117	-0.3581
H	-4.3433	-3.0874	1.3420
C	-2.8921	-2.1414	-2.8404
O	-3.6184	-3.1293	-2.9114
N	-1.5750	-2.1549	-2.5386
H	-3.2629	-1.1243	-3.0388
C	-0.7981	-0.9316	-2.5232
H	0.0354	-1.0050	-3.2327
H	-1.4311	-0.0927	-2.8252
H	-0.3876	-0.7401	-1.5252
C	-0.8772	-3.3948	-2.2759
H	-1.6076	-4.2016	-2.2037
H	-0.1674	-3.6210	-3.0817
H	-0.3208	-3.3196	-1.3356
C	-7.0436	1.1356	-2.9976
O	-7.7368	2.1446	-3.1197
N	-6.8308	0.2151	-3.9615
H	-6.5186	0.8935	-2.0599
C	-6.0227	-0.9642	-3.7197
H	-5.1773	-0.9921	-4.4144
H	-5.6377	-0.9437	-2.6974
H	-6.6209	-1.8733	-3.8568
C	-7.4100	0.3660	-5.2783
H	-7.9700	1.3011	-5.3118
H	-6.6219	0.3848	-6.0406
H	-8.0859	-0.4691	-5.5006

Cluster-7_DMF

Energy(POTENTIAL) = -1739.14073511

Atom	X	Y	Z
C	-0.9936	2.2339	-0.4222
O	-2.1046	2.6507	-0.0945
N	-0.3060	2.6140	-1.5171
H	-0.4525	1.4842	0.1771
C	1.0077	2.0713	-1.8036
H	1.7613	2.8679	-1.7933
H	1.2653	1.3237	-1.0491
H	1.0162	1.5997	-2.7931
C	-0.8254	3.6097	-2.4320
H	-1.7768	3.9812	-2.0501
H	-0.1189	4.4433	-2.5192
H	-0.9752	3.1725	-3.4258
C	1.2016	-1.4835	0.8598
O	1.0365	-0.2726	0.7214
N	1.9206	-2.2766	0.0442
H	0.7461	-2.0355	1.6982
C	2.1238	-3.6819	0.3370
H	1.8425	-4.2917	-0.5291
H	3.1768	-3.8771	0.5717
H	1.5089	-3.9785	1.1901
C	2.6200	-1.7433	-1.1075
H	2.3511	-0.6961	-1.2434
H	3.7042	-1.8223	-0.9634
H	2.3447	-2.3085	-2.0047
C	-3.4629	1.7749	-3.1438
O	-2.9963	1.0561	-4.0302
N	-4.2566	2.8388	-3.3473
H	-3.2488	1.6002	-2.0805
C	-4.7128	3.6624	-2.2441
H	-5.8050	3.6197	-2.1718
H	-4.2647	3.3073	-1.3134
H	-4.4088	4.7039	-2.4029
C	-4.6740	3.2178	-4.6811
H	-4.4007	2.4244	-5.3778
H	-5.7593	3.3579	-4.6933
H	-4.1868	4.1518	-4.9876
C	-3.8482	-0.2729	-0.0705
O	-4.9347	0.0464	-0.5504
N	-3.4822	-1.5264	0.2605
H	-3.0701	0.4781	0.1403
C	-2.1876	-1.8089	0.8434
H	-1.6443	-2.5336	0.2268
H	-1.5980	-0.8910	0.9092
H	-2.3028	-2.2286	1.8502
C	-4.3875	-2.6439	0.0869
H	-5.3445	-2.2671	-0.2758
H	-3.9823	-3.3545	-0.6416
H	-4.5368	-3.1560	1.0446
C	-2.6675	-2.1155	-2.9252
O	-3.3156	-3.1428	-3.1148
N	-1.3813	-2.0697	-2.5135
H	-3.0899	-1.1127	-3.0908
C	-0.6994	-0.8065	-2.3141
H	0.2341	-0.7898	-2.8893
H	-1.3350	0.0097	-2.6673
H	-0.4531	-0.6539	-1.2572
C	-0.6251	-3.2826	-2.2897
H	-1.3083	-4.1326	-2.3061

H	0.1363	−3.4167	−3.0692
H	−0.1226	−3.2341	−1.3182
C	−6.8675	1.1604	−3.1170
O	−7.5411	2.1639	−3.3484
N	−6.5856	0.1898	−4.0094
H	−6.4112	0.9739	−2.1315
C	−5.8859	−1.0188	−3.6164
H	−5.0780	−1.2304	−4.3207
H	−5.4687	−0.8924	−2.6144
H	−6.5703	−1.8779	−3.6118
C	−7.0885	0.2546	−5.3664
H	−7.4122	1.2747	−5.5773
H	−6.2962	−0.0431	−6.0615
H	−7.9416	−0.4243	−5.5007
C	−3.3460	−0.9638	−6.4635
O	−4.4100	−1.4119	−6.8861
N	−2.2378	−1.6921	−6.2151
H	−3.2090	0.1036	−6.2367
C	−1.0005	−1.0673	−5.7944
H	−0.2754	−1.0342	−6.6176
H	−1.1994	−0.0533	−5.4404
H	−0.5615	−1.6416	−4.9727
C	−2.2230	−3.1255	−6.4137
H	−3.1852	−3.4320	−6.8253
H	−1.4237	−3.4066	−7.1094
H	−2.0620	−3.6361	−5.4570

Cluster-8_DMF

Energy(POTENTIAL) = −1987.58958653

Atom	X	Y	Z
C	−1.0861	2.3706	−0.2974
O	−2.2499	2.6658	−0.0235
N	−0.3953	2.8209	−1.3630
H	−0.4946	1.6874	0.3326
C	0.9824	2.4272	−1.5862
H	1.6424	3.3021	−1.5416
H	1.2871	1.7093	−0.8206
H	1.0895	1.9642	−2.5741
C	−0.9790	3.7521	−2.3068
H	−1.9772	4.0255	−1.9639
H	−0.3609	4.6549	−2.3752
H	−1.0465	3.2976	−3.3019
C	1.3812	−1.0646	1.1407
O	1.1486	0.1281	0.9521
N	2.1687	−1.8415	0.3734
H	0.9387	−1.6115	1.9891
C	2.4448	−3.2218	0.7211
H	2.1988	−3.8804	−0.1198
H	3.5055	−3.3518	0.9655
H	1.8436	−3.5159	1.5848
C	2.8646	−1.3051	−0.7792
H	2.5197	−0.2887	−0.9685
H	3.9464	−1.2929	−0.6003
H	2.6622	−1.9268	−1.6580
C	−3.4268	1.6899	−3.1262
O	−2.8958	0.9869	−3.9883
N	−4.2779	2.7010	−3.3648
H	−3.2248	1.5462	−2.0553
C	−4.8158	3.5072	−2.2858
H	−5.9042	3.3928	−2.2392
H	−4.3685	3.1964	−1.3387
H	−4.5773	4.5642	−2.4534
C	−4.6838	3.0362	−4.7137
H	−4.3368	2.2579	−5.3943
H	−5.7757	3.1002	−4.7575
H	−4.2546	3.9993	−5.0167
C	−3.8408	−0.3532	−0.0385
O	−4.9597	−0.2347	−0.5354
N	−3.2719	−1.5199	0.3243
H	−3.2008	0.5222	0.1602
C	−1.9626	−1.5660	0.9399
H	−1.3004	−2.2246	0.3669
H	−1.5240	−0.5658	0.9677
H	−2.0314	−1.9510	1.9648
C	−3.9726	−2.7785	0.1733
H	−4.9434	−2.5883	−0.2850
H	−3.3992	−3.4545	−0.4691
H	−4.1177	−3.2505	1.1526
C	−2.2702	−2.0860	−2.7941
O	−2.8210	−3.1773	−2.9492
N	−1.0049	−1.9159	−2.3646
H	−2.7783	−1.1355	−3.0102
C	−0.4376	−0.5923	−2.1946
H	0.4906	−0.5051	−2.7716
H	−1.1445	0.1560	−2.5612
H	−0.2069	−0.4013	−1.1405
C	−0.1523	−3.0498	−2.0770
H	−0.7552	−3.9585	−2.0746
H	0.6367	−3.1424	−2.8340
H	0.3176	−2.9190	−1.0973
C	−6.7754	0.8625	−3.2060
O	−7.5271	1.8092	−3.4385
N	−6.3705	−0.0508	−4.1101
H	−6.3457	0.6862	−2.2064
C	−5.5704	−1.1994	−3.7252
H	−4.6617	−1.2422	−4.3318
H	−5.2931	−1.1157	−2.6714
H	−6.1343	−2.1271	−3.8837
C	−6.8210	0.0095	−5.4855
H	−7.2193	1.0049	−5.6868
H	−5.9812	−0.2078	−6.1539
H	−7.6100	−0.7325	−5.6704
C	−3.0294	−0.8911	−6.5150
O	−4.0493	−1.3801	−6.9947
N	−1.9476	−1.5907	−6.1123
H	−2.9167	0.1911	−6.3533
C	−0.7258	−0.9194	−5.7181
H	0.0120	−0.9258	−6.5310
H	−0.9471	0.1116	−5.4342
H	−0.2900	−1.4307	−4.8546
C	−1.9074	−3.0315	−6.2464
H	−2.9247	−3.4024	−6.3792
H	−1.2990	−3.3335	−7.1092
H	−1.4790	−3.4697	−5.3404
C	−5.2216	−4.6211	−4.7327
O	−6.4047	−4.3636	−4.9391
N	−4.5422	−5.6488	−5.2922
H	−4.5917	−4.0146	−4.0618
C	−3.1795	−5.9535	−4.9052
H	−2.5217	−5.9574	−5.7828
H	−2.8217	−5.2033	−4.1953
H	−3.1279	−6.9429	−4.4330
C	−5.1938	−6.5614	−6.2072

H	-6.1774	-6.1626	-6.4580
H	-4.5991	-6.6665	-7.1217
H	-5.3116	-7.5530	-5.7519

4a_DMF

Energy(POTENTIAL) = -1596.59237767

Atom	X	Y	Z
Ag	4.1264	11.9452	1.6233
C	2.8366	13.1597	0.4797
C	3.8266	8.6679	1.7141
C	4.1703	7.3339	1.9959
H	3.5480	6.5344	1.6071
C	5.3011	7.0359	2.7299
C	6.0885	8.1175	3.2170
C	5.6809	9.4237	2.8776
N	4.5775	9.6762	2.1393
C	7.2328	7.9429	4.0651
H	7.5034	6.9439	4.3870
C	7.9621	9.0036	4.4892
H	8.8094	8.8438	5.1463
C	6.4639	10.5629	3.3325
C	7.6190	10.3442	4.1095
C	8.3637	11.4865	4.5178
C	7.8856	12.7329	4.1685
H	8.4273	13.6259	4.4631
C	6.7140	12.8651	3.4016
N	6.0361	11.8001	2.9905
C	2.6041	8.9990	0.9081
H	1.9212	9.6228	1.4952
H	2.0738	8.0937	0.6016
H	2.8798	9.5646	0.0112
C	5.6521	5.6131	2.9774
C	4.6962	4.7440	3.5155
H	3.7170	5.1276	3.7891
C	4.9980	3.3997	3.7151
H	4.2497	2.7371	4.1400
C	6.2544	2.9059	3.3694
H	6.4878	1.8564	3.5228
C	7.2086	3.7631	2.8242
H	8.1865	3.3828	2.5436
C	6.9118	5.1089	2.6303
H	7.6557	5.7687	2.1925
C	9.6232	11.3802	5.2992
C	10.7013	10.6218	4.8269
H	10.6135	10.0891	3.8841
C	11.8902	10.5653	5.5481
H	12.7224	9.9807	5.1671
C	12.0141	11.2585	6.7509
H	12.9419	11.2103	7.3135
C	10.9455	12.0156	7.2268
H	11.0347	12.5557	8.1648
C	9.7579	12.0807	6.5029
H	8.9242	12.6684	6.8772
C	6.2098	14.2187	2.9936
H	6.3074	14.3466	1.9093
H	6.7710	15.0165	3.4867
H	5.1494	14.3262	3.2444
F	1.5319	12.7065	0.3688
F	3.2198	13.3242	-0.8411
F	2.6713	14.4635	0.9181

4a'_DMF

Energy(POTENTIAL) = -3193.24580396

Atom	X	Y	Z
Ag	3.8792	12.3794	3.0487
C	2.5643	13.2480	1.6392
N	5.8381	12.3587	4.3215
F	2.6170	14.6235	1.4804
F	1.2129	13.0106	1.8201
F	2.7810	12.7875	0.3435
N	4.5072	10.1310	3.5847
C	6.5096	13.4722	4.5903
C	6.3025	11.1739	4.7801
C	3.8470	9.0670	3.1498
C	5.5747	9.9726	4.3934
C	5.9565	14.7655	4.0687
C	7.7119	13.4382	5.3133
C	7.4609	11.0632	5.5763
C	2.6839	9.2910	2.2273
C	4.2403	7.7713	3.5171
C	6.0148	8.7109	4.8431
H	4.9541	14.9407	4.4730
H	5.8670	14.7260	2.9769
H	6.5977	15.6089	4.3378
C	8.2182	12.2499	5.8068
H	8.2591	14.3646	5.4509
C	7.7900	9.7773	6.1267
H	1.9976	10.0363	2.6415
H	3.0374	9.6711	1.2616
H	2.1342	8.3625	2.0524
C	5.3180	7.5655	4.3586
H	3.6992	6.9239	3.1095
C	7.1007	8.6612	5.7821
C	9.5348	12.2697	6.4970
H	8.5911	9.7054	6.8536
C	5.6947	6.1666	4.6854
H	7.3635	7.7126	6.2352
C	9.8472	13.3220	7.3689
C	10.5174	11.3061	6.2325
C	4.6922	5.2385	4.9993
C	7.0215	5.7261	4.6088
C	11.0948	13.3987	7.9768
H	9.1020	14.0812	7.5828
C	11.7677	11.3847	6.8405
H	10.3188	10.5075	5.5244
C	5.0077	3.9053	5.2338
H	3.6600	5.5683	5.0764
C	7.3367	4.3913	4.8503
H	7.8082	6.4207	4.3298
C	12.0592	12.4272	7.7174
H	11.3090	14.2122	8.6636
H	12.5182	10.6318	6.6189
C	6.3324	3.4778	5.1622
H	4.2198	3.2027	5.4876
H	8.3699	4.0637	4.7801
H	13.0325	12.4829	8.1957
H	6.5798	2.4370	5.3498
Ag	3.3385	12.6022	6.4064
C	2.0613	14.1256	5.6784
F	2.6121	15.0980	4.8543

F	0.9482	13.7148	4.9632
F	1.5014	14.8849	6.6984
N	3.6784	10.3677	7.0157
N	5.1882	12.4435	7.9158
H	7.6050	14.1789	9.4487
C	5.8939	13.4821	8.3445
C	7.0179	13.3097	9.1709
C	7.4050	12.0499	9.5814
C	6.5828	10.9495	9.2124
C	5.5027	11.2018	8.3436
C	4.6785	10.0938	7.8857
C	4.9402	8.7920	8.3591
C	5.9721	8.6024	9.3376
C	6.7664	9.6258	9.7307
C	4.1380	7.7288	7.8557
C	3.1229	8.0503	6.9764
C	2.9016	9.3821	6.5824
H	6.1050	7.6251	9.7849
H	10.4462	13.2598	12.8885
H	7.5292	9.4547	10.4814
H	4.4137	15.0146	8.1044
H	5.6120	14.9555	6.8094
H	6.0596	15.6285	8.3879
C	5.4751	14.8500	7.8906
H	9.3797	10.2626	9.0896
H	11.5335	10.0350	10.2642
H	12.0818	11.5340	12.1692
C	8.9905	12.7226	11.4028
C	10.2115	12.5978	12.0600
C	11.1282	11.6281	11.6581
C	10.8183	10.7821	10.5950
C	9.5983	10.9039	9.9388
C	8.6691	11.8735	10.3378
C	1.7653	9.7299	5.6667
H	8.2766	13.4761	11.7242
C	4.3605	6.3104	8.2375
H	0.9171	10.1030	6.2544
H	2.0577	10.5192	4.9681
H	1.4289	8.8564	5.1014
H	2.4917	7.2716	6.5613
C	3.2673	5.5072	8.5833
C	5.6389	5.7372	8.2121
C	3.4493	4.1658	8.9082
H	2.2713	5.9401	8.6127
C	5.8196	4.3983	8.5414
H	6.4943	6.3316	7.9066
C	4.7261	3.6087	8.8920
H	2.5913	3.5578	9.1802
H	6.8154	3.9670	8.5060
H	4.8685	2.5621	9.1446

4b-ani_DMF

Energy(POTENTIAL) = -822.21154700

Atom	X	Y	Z
Ag	4.2854	12.0291	1.4136
C	2.8196	13.0829	0.3296
F	1.9497	12.2995	-0.4073
F	3.3120	13.9721	-0.6095
F	1.9679	13.8670	1.0865
C	5.7544	10.9728	2.4909
F	6.1714	9.7870	1.9131
F	5.3878	10.5870	3.7678
F	6.9411	11.6529	2.6985

4b-cat-I_DMF

Energy(POTENTIAL) = -2370.97819770

Atom	X	Y	Z
Ag	4.1983	12.0700	1.8912
C	3.8194	8.8037	1.9086
C	4.1350	7.4600	2.1761
H	3.4751	6.6780	1.8144
C	5.2857	7.1324	2.8650
C	6.1243	8.1903	3.3174
C	5.7404	9.5091	2.9983
N	4.6138	9.7881	2.3066
C	7.3006	7.9779	4.1107
H	7.5573	6.9692	4.4134
C	8.0786	9.0152	4.5046
H	8.9518	8.8275	5.1189
C	6.5745	10.6253	3.4247
C	7.7574	10.3675	4.1469
C	8.5568	11.4834	4.5254
C	8.1022	12.7473	4.2096
H	8.6854	13.6207	4.4832
C	6.9009	12.9207	3.4996
N	6.1734	11.8804	3.1125
C	2.5807	9.1789	1.1473
H	1.9420	9.8285	1.7571
H	2.0059	8.2948	0.8602
H	2.8445	9.7347	0.2400
C	5.6077	5.7011	3.1042
C	4.6656	4.8682	3.7179
H	3.7197	5.2845	4.0534
C	4.9406	3.5174	3.9140
H	4.2045	2.8832	4.3992
C	6.1549	2.9820	3.4891
H	6.3674	1.9276	3.6400
C	7.0946	3.8035	2.8689
H	8.0389	3.3905	2.5266
C	6.8254	5.1558	2.6790
H	7.5571	5.7891	2.1850
C	9.8536	11.3259	5.2339
C	10.8740	10.5359	4.6903
H	10.7131	10.0217	3.7468
C	12.0976	10.4209	5.3430
H	12.8836	9.8104	4.9085
C	12.3140	11.0881	6.5477
H	13.2676	10.9926	7.0587
C	11.3046	11.8790	7.0926
H	11.4662	12.4000	8.0317
C	10.0821	12.0023	6.4373
H	9.2943	12.6156	6.8661
C	6.4204	14.2889	3.1132
H	6.5618	14.4450	2.0368
H	6.9687	15.0702	3.6460
H	5.3513	14.3969	3.3264
C	4.1438	12.9139	-1.2668
C	3.6293	13.4442	-2.4626
H	4.1964	13.3308	-3.3806
C	2.4014	14.0752	-2.4820

C	1.6874	14.1944	-1.2562
C	2.2648	13.6201	-0.1052
N	3.4659	12.9986	-0.1294
C	0.4429	14.8985	-1.1349
H	0.0362	15.4021	-2.0044
C	-0.2184	14.9626	0.0462
H	-1.1471	15.5177	0.1099
C	1.5526	13.6867	1.1642
C	0.2977	14.3269	1.2249
C	-0.3755	14.3396	2.4794
C	0.2554	13.7634	3.5643
H	-0.2311	13.7521	4.5341
C	1.5175	13.1612	3.4221
N	2.1327	13.1237	2.2476
C	5.4744	12.2202	-1.2285
H	6.1721	12.7788	-0.5936
H	5.9097	12.1322	-2.2272
H	5.3687	11.2168	-0.8002
C	1.8705	14.5950	-3.7691
C	2.6534	15.4524	-4.5502
H	3.6295	15.7651	-4.1892
C	2.1815	15.9177	-5.7747
H	2.7956	16.5885	-6.3683
C	0.9277	15.5227	-6.2368
H	0.5601	15.8849	-7.1925
C	0.1463	14.6608	-5.4690
H	-0.8277	14.3415	-5.8282
C	0.6128	14.1998	-4.2413
H	0.0042	13.5197	-3.6517
C	-1.7202	14.9474	2.6569
C	-2.8057	14.5447	1.8693
H	-2.6663	13.7840	1.1060
C	-4.0656	15.1007	2.0712
H	-4.9006	14.7762	1.4571
C	-4.2557	16.0664	3.0583
H	-5.2381	16.5038	3.2106
C	-3.1813	16.4682	3.8492
H	-3.3215	17.2207	4.6197
C	-1.9215	15.9087	3.6537
H	-1.0838	16.2281	4.2676
C	2.2151	12.5198	4.5863
H	2.3869	11.4556	4.3869
H	1.6312	12.6135	5.5054
H	3.1943	12.9864	4.7447

4b-cat-II_DMF

Energy(POTENTIAL) = -2867.89993197

Atom	X	Y	Z
Ag	7.5739	10.5406	-0.3801
C	5.8098	12.2243	-3.7551
C	5.9932	13.5847	-4.0672
H	6.3325	13.8558	-5.0625
C	5.7154	14.5654	-3.1364
C	5.2504	14.1480	-1.8528
C	5.0460	12.7647	-1.6518
N	5.3376	11.8315	-2.5854
C	5.0181	15.0438	-0.7544
H	5.2966	16.0868	-0.8552
C	4.4767	14.6086	0.4112
H	4.3294	15.3120	1.2233
C	4.4788	12.2945	-0.3915
C	4.1195	13.2308	0.6034
C	3.4550	12.7342	1.7657
C	3.2835	11.3686	1.8705
H	2.7701	10.9454	2.7285
C	3.7439	10.5058	0.8576
N	4.3098	10.9611	-0.2461
C	6.1141	11.1678	-4.7807
H	5.3103	11.1187	-5.5258
H	6.2015	10.1872	-4.3055
H	7.0424	11.3910	-5.3164
C	5.8859	15.9888	-3.5328
C	7.0107	16.3704	-4.2771
H	7.7785	15.6366	-4.5015
C	7.1633	17.6791	-4.7207
H	8.0508	17.9558	-5.2823
C	6.1918	18.6338	-4.4277
H	6.3129	19.6585	-4.7667
C	5.0645	18.2661	-3.6962
H	4.2950	18.9997	-3.4747
C	4.9091	16.9540	-3.2558
H	4.0081	16.6755	-2.7175
C	2.9085	13.6062	2.8397
C	2.1772	14.7638	2.5426
H	2.0188	15.0540	1.5083
C	1.6168	15.5296	3.5618
H	1.0500	16.4218	3.3116
C	1.7702	15.1482	4.8929
H	1.3356	15.7487	5.6867
C	2.4848	13.9921	5.1999
H	2.6188	13.6910	6.2347
C	3.0478	13.2295	4.1827
H	3.6122	12.3367	4.4333
C	3.5568	9.0200	0.9893
H	2.5223	8.7453	0.7472
H	3.7534	8.6841	2.0122
H	4.2201	8.4883	0.3021
C	8.8375	13.1332	-1.9674
C	9.1333	14.4845	-2.2225
H	9.5409	14.7595	-3.1895
C	8.8754	15.4528	-1.2748
C	8.3530	15.0318	-0.0186
C	8.0428	13.6660	0.1421
N	8.2802	12.7523	-0.8271
C	8.1750	15.9242	1.0878
H	8.5074	16.9515	0.9984
C	7.6333	15.4973	2.2527
H	7.5382	16.1885	3.0817
C	7.4602	13.2062	1.3955
C	7.2176	14.1372	2.4252
C	6.6084	13.6629	3.6222
C	6.3838	12.3082	3.7354
H	5.9300	11.8993	4.6321
C	6.6900	11.4366	2.6729
N	7.1847	11.8869	1.5302
C	9.1565	12.0769	-2.9841
H	10.1176	11.6073	-2.7385
H	9.2360	12.5016	-3.9884
H	8.3943	11.2925	-2.9834
C	9.1244	16.8814	-1.5940
C	10.3212	17.2653	-2.2092
H	11.0887	16.5209	-2.4024
C	10.5414	18.5947	-2.5591

H	11.4778	18.8783	-3.0304
C	9.5669	19.5569	-2.3021
H	9.7394	20.5943	-2.5735
C	8.3687	19.1821	-1.6968
H	7.5964	19.9221	-1.5096
C	8.1465	17.8541	-1.3486
H	7.1957	17.5669	-0.9090
C	6.1899	14.5758	4.7152
C	5.4423	15.7276	4.4372
H	5.1763	15.9642	3.4109
C	5.0057	16.5515	5.4688
H	4.4189	17.4356	5.2375
C	5.3036	16.2336	6.7926
H	4.9611	16.8771	7.5977
C	6.0390	15.0852	7.0793
H	6.2746	14.8322	8.1089
C	6.4786	14.2603	6.0475
H	7.0589	13.3701	6.2750
C	6.4605	9.9635	2.8305
H	5.5545	9.7678	3.4115
H	7.3028	9.5124	3.3700
H	6.3741	9.4705	1.8578
C	8.3344	7.7313	-1.4108
O	7.3765	8.5286	-1.3586
N	8.3266	6.6094	-2.1256
H	9.2551	7.9233	-0.8473
C	9.4732	5.7187	-2.1403
H	9.8694	5.6317	-3.1576
H	10.2544	6.1084	-1.4845
H	9.1781	4.7240	-1.7899
C	7.1802	6.2197	-2.9270
H	6.4184	6.9967	-2.8720
H	7.4880	6.0826	-3.9687
H	6.7673	5.2766	-2.5533
C	9.8294	9.6762	1.8226
O	9.9419	9.6022	0.5938
N	10.0950	10.7618	2.5613
H	9.4867	8.8159	2.4180
C	9.9568	10.7554	4.0043
H	9.2052	11.4899	4.3161
H	9.6483	9.7651	4.3475
H	10.9121	11.0090	4.4771
C	10.5821	11.9833	1.9506
H	10.3902	11.9526	0.8781
H	10.0658	12.8427	2.3886
H	11.6590	12.0967	2.1249

Bc-Ligand_DMF

Energy(POTENTIAL) = -1112.00363093

Atom	X	Y	Z
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C	3.5090	13.4456	-2.5496
H	4.0780	13.3571	-3.4707
C	2.3447	14.1809	-2.5228
C	1.6316	14.2589	-1.2903
C	2.1605	13.5598	-0.1820
N	3.3034	12.8363	-0.2439
C	0.4437	15.0450	-1.1238
H	0.0771	15.6316	-1.9589
C	-0.2143	15.0836	0.0613
H	-1.1026	15.6978	0.1606
C	1.4633	13.6180	1.0984
C	0.2588	14.3494	1.1987
C	-0.4056	14.3595	2.4604
C	0.1944	13.7035	3.5122
H	-0.2791	13.6885	4.4897
C	1.4156	13.0213	3.3219
N	2.0191	12.9683	2.1482
C	5.2292	11.9754	-1.4337
H	6.0852	12.6134	-1.6837
H	5.1703	11.1969	-2.2029
H	5.4123	11.5034	-0.4654
C	1.8890	14.8723	-3.7589
C	2.7592	15.7473	-4.4192
H	3.7443	15.9364	-4.0013
C	2.3661	16.3850	-5.5927
H	3.0496	17.0674	-6.0897
C	1.1002	16.1503	-6.1255
H	0.7928	16.6473	-7.0409
C	0.2302	15.2734	-5.4794
H	-0.7548	15.0798	-5.8941
C	0.6202	14.6386	-4.3034
H	-0.0590	13.9484	-3.8106
C	-1.7098	15.0433	2.6689
C	-2.8249	14.7166	1.8875
H	-2.7333	13.9670	1.1062
C	-4.0516	15.3332	2.1162
H	-4.9100	15.0657	1.5067
C	-4.1791	16.2863	3.1254
H	-5.1355	16.7705	3.2999
C	-3.0752	16.6146	3.9097
H	-3.1662	17.3579	4.6965
C	-1.8488	15.9937	3.6864
H	-0.9878	16.2554	4.2957
C	2.0681	12.3164	4.4790
H	1.3959	11.5652	4.9093
H	2.3130	13.0276	5.2766
H	2.9865	11.8234	4.1513

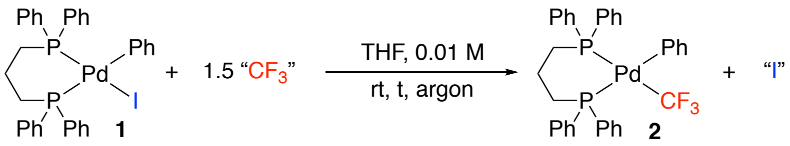
4b-ionpair_DMF

Energy(POTENTIAL) = -3441.68688851

Atom	X	Y	Z
Ag	6.9221	10.4708	-0.0086
C	5.7094	12.3535	-3.8751
C	5.9634	13.7047	-4.1794
H	6.3493	13.9617	-5.1614
C	5.7025	14.6947	-3.2546
C	5.1778	14.2993	-1.9876
C	4.9269	12.9244	-1.7872
N	5.1982	11.9808	-2.7158
C	4.9361	15.2087	-0.9033
H	5.2353	16.2454	-1.0065
C	4.3471	14.7975	0.2476
H	4.1896	15.5117	1.0480
C	4.3352	12.4761	-0.5305
C	3.9601	13.4283	0.4427
C	3.2516	12.9560	1.5883
C	3.0665	11.5927	1.7112
H	2.5184	11.1886	2.5566
C	3.5630	10.7096	0.7348

N	4.1689	11.1446	-0.3590
C	5.9940	11.2856	-4.8936
H	5.2333	11.3009	-5.6839
H	5.9818	10.2985	-4.4247
H	6.9658	11.4441	-5.3724
C	5.9676	16.1075	-3.6345
C	7.1607	16.4329	-4.2940
H	7.9074	15.6623	-4.4617
C	7.4058	17.7330	-4.7222
H	8.3415	17.9667	-5.2214
C	6.4618	18.7328	-4.4956
H	6.6546	19.7504	-4.8226
C	5.2696	18.4207	-3.8459
H	4.5223	19.1906	-3.6773
C	5.0210	17.1174	-3.4224
H	4.0736	16.8820	-2.9464
C	2.6758	13.8584	2.6205
C	1.9853	15.0259	2.2670
H	1.8718	15.2917	1.2204
C	1.4117	15.8346	3.2442
H	0.8790	16.7343	2.9503
C	1.5093	15.4869	4.5900
H	1.0681	16.1229	5.3518
C	2.1744	14.3174	4.9516
H	2.2625	14.0400	5.9980
C	2.7493	13.5104	3.9759
H	3.2751	12.6077	4.2698
C	3.3789	9.2245	0.8778
H	2.4492	8.9112	0.3862
H	3.3186	8.9258	1.9280
H	4.2051	8.6915	0.3989
C	8.4981	12.9050	-1.6698
C	8.8726	14.2293	-1.9650
H	9.2886	14.4506	-2.9424
C	8.6840	15.2371	-1.0433
C	8.1397	14.8849	0.2254
C	7.7456	13.5448	0.4251
N	7.9213	12.5921	-0.5193
C	8.0117	15.8210	1.3017
H	8.4074	16.8224	1.1827
C	7.4371	15.4649	2.4746
H	7.3760	16.1863	3.2809
C	7.1351	13.1586	1.6910
C	6.9459	14.1367	2.6884
C	6.3128	13.7413	3.9020
C	6.0066	12.4093	4.0611
H	5.5329	12.0599	4.9729
C	6.2432	11.4860	3.0250
N	6.7671	11.8635	1.8675
C	8.7617	11.8092	-2.6607
H	9.7518	11.3755	-2.4748
H	8.7556	12.1947	-3.6840
H	8.0201	11.0101	-2.5748
C	9.0275	16.6371	-1.4029
C	10.2421	16.9195	-2.0379
H	10.9553	16.1191	-2.2149
C	10.5503	18.2205	-2.4273
H	11.5000	18.4244	-2.9132
C	9.6477	19.2551	-2.1907
H	9.8881	20.2697	-2.4947
C	8.4321	18.9819	-1.5659
H	7.7141	19.7781	-1.3941
C	8.1227	17.6829	-1.1773
H	7.1622	17.4775	-0.7155
C	5.9484	14.7109	4.9657
C	5.2256	15.8704	4.6569
H	4.9486	16.0763	3.6268
C	4.8271	16.7423	5.6648
H	4.2575	17.6316	5.4110
C	5.1431	16.4669	6.9939
H	4.8308	17.1480	7.7801
C	5.8574	15.3129	7.3107
H	6.1061	15.0927	8.3447
C	6.2552	14.4380	6.3035
H	6.8155	13.5411	6.5533
C	5.8820	10.0473	3.2339
H	4.9024	9.9588	3.7150
H	6.6151	9.5697	3.8940
H	5.8655	9.4986	2.2903
C	8.0729	7.9979	-1.2732
O	6.9771	8.5973	-1.2820
N	8.2074	6.6761	-1.2471
H	9.0215	8.5472	-1.2982
C	9.5194	6.0554	-1.1849
H	9.6512	5.3716	-2.0296
H	10.2967	6.8217	-1.2184
H	9.6153	5.4912	-0.2515
C	7.0579	5.7914	-1.1831
H	6.1438	6.3788	-1.2582
H	7.1021	5.0724	-2.0072
H	7.0667	5.2491	-0.2337
Ag	8.8336	8.4668	1.8238
C	10.2769	9.9114	1.2848
F	10.4277	10.1608	-0.0735
F	11.5651	9.5849	1.6747
F	10.1061	11.1772	1.8161
C	7.4917	6.9397	2.4018
F	6.2314	6.9556	1.8322
F	7.2150	6.8894	3.7581
F	7.9349	5.6514	2.1332

Transmetalation studies in the benchmark system



- **Procedure for R_3SiCF_3 (R = Me or Et)/MF (M = K or Cs)**

Inside the glovebox, a 5 mL-crimped vial containing a 12mmx3mm PTFE cylindrical stirrer was charged with Pd complex **1** (4.3 mg, 0.006 mmol) and CsF (1.4 mg, 0.009 mmol) or KF (0.5 mg, 0.009 mmol) and dissolved in 0.5 mL of THF. After that, Me_3SiCF_3 or Et_3SiCF_3 (100 μL of a 0.09 M stock solution in THF) were added and the heterogeneous mixture was left stirring at 1500 rpm the corresponding time at room temperature.

- **Procedure for (Phen)$CuCF_3$**

Inside the glovebox, a 5 mL-crimped vial containing a 12mmx3mm PTFE cylindrical stirrer was charged with Pd complex **1** (4.3 mg, 0.006 mmol) and (Phen)$CuCF_3$ (2.8 mg, 0.009 mmol) and dissolved in 0.6 mL of THF. The heterogeneous mixture was left stirring at 1500 rpm the corresponding time at room temperature.

- **Procedure for complexes 3 and 4**

Outside the glovebox, a 5 mL-crimped vial containing a 12mmx3mm PTFE cylindrical stirrer was charged with Pd complex **1** (4.3 mg, 0.006 mmol) and **3** (5.1 mg, 0.009 mmol) or **4** (4.8 mg, 0.009 mmol), purged under argon, dissolved in 0.6 mL of THF and left stirring at 1500 rpm the corresponding time at room temperature.

- **Procedure for complexes 8**

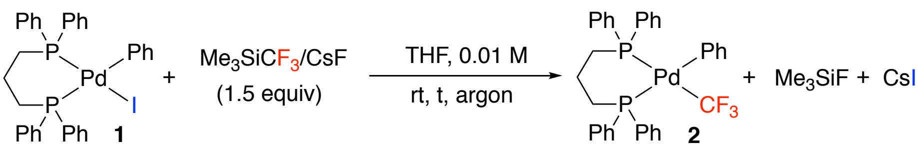
"CF_3" sources [1.7 mg (**8**$_{Cs}$), 2.2 mg (**8**$_{NBu_4}$), 0.0045 mmol] and Pd complex **1** (4.3 mg, 0.006 mmol) were weighted in a 5 mL-crimped vial containing a 12mmx3mm PTFE cylindrical stirrer inside the glovebox, dissolved in 0.6 mL of THF and left stirring at 1500 rpm the corresponding time at room temperature.

After that, for all the procedures, the reactions were cooled at –80 ºC and transferred to different NMR tubes previously purged and cooled. All the ^{19}F (ns = 256 scans) and $^{31}P\{^1H\}$ (ns = 1024 scans) NMR experiments were measured at –80 ºC and each reaction was repeated at least three times, taking the average for the percentage of the product formed determined by $^{31}P\{^1H\}$ NMR. The NMR data is in accordance with the previously described (dppp)Pd(Ph)(CF_3),[4] the excess of the corresponding "$AgCF_3$" source and the different observed intermediates when it is the case.

Table S7. % conversion of (dppp)Pd(Ph)(CF_3) product using different CF_3 sources

	% product (dppp)Pd(Ph)(CF_3)							
t (min)	Me_3SiCF_3/CsF	Et_3SiCF_3/CsF	Et_3SiCF_3/KF	(Phen)$CuCF_3$	**3**	**4**	**8**$_{Cs}$	**8**$_{NBu_4}$
10	0	0	0	12	0	100	100	93
30	19	traces	0	-	4	-	-	-

- **Transmetalation between complex 1 and Me_3SiCF_3/CsF**



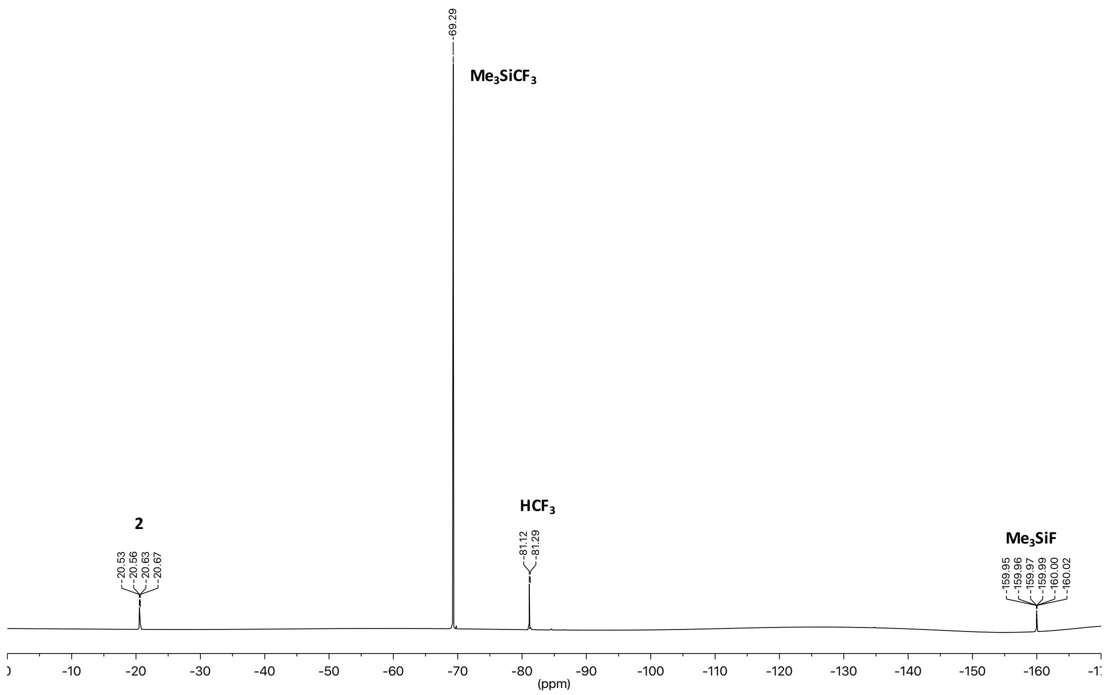


Figure S20. ^{19}F NMR spectrum of the reaction of **1** and Me_3SiCF_3/CsF after 30 min measured at –80 ºC.

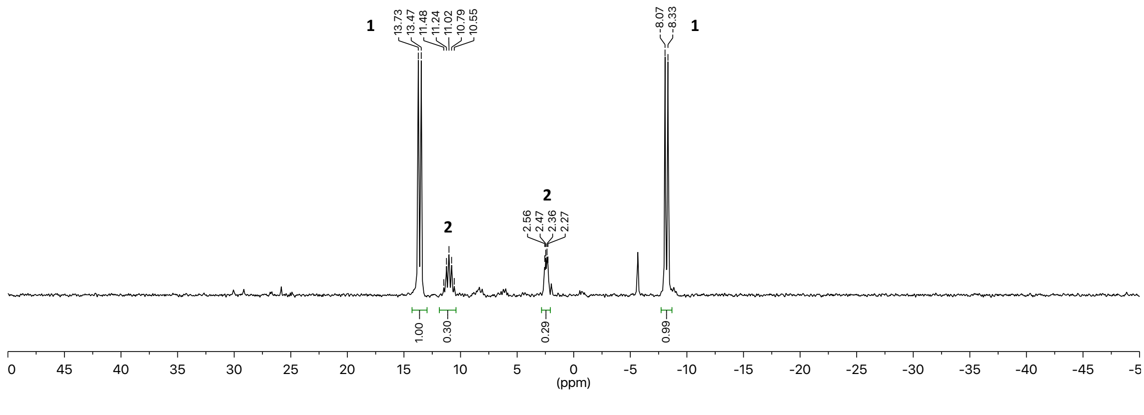
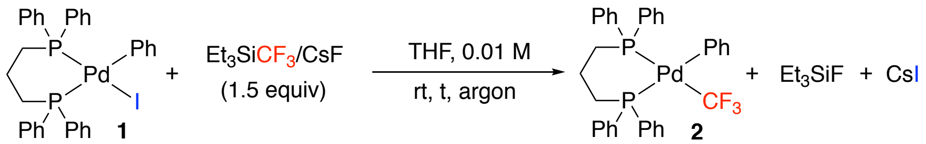


Figure S21. $^{31}P\{^1H\}$ NMR spectrum of the reaction of **1** and Me_3SiCF_3/CsF after 30 min measured at –80 ºC.

- **Transmetalation between complex 1 and Et_3SiCF_3/CsF**



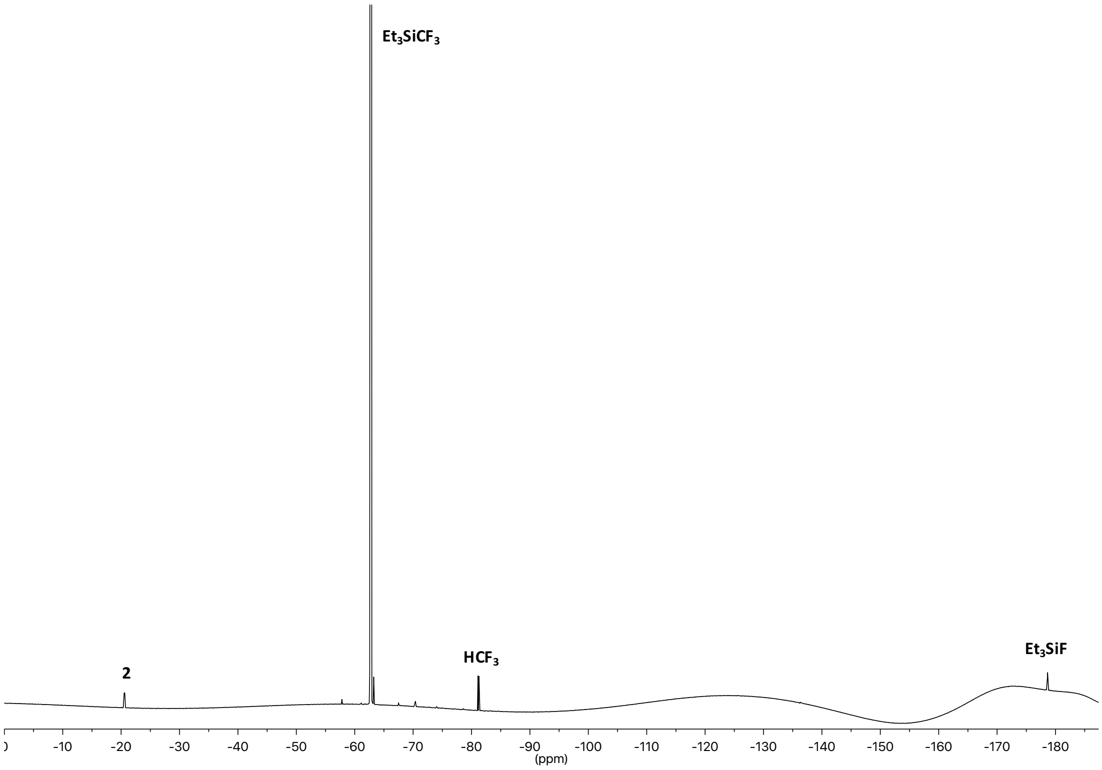


Figure S22. ^{19}F NMR spectrum of the reaction of **1** and Et_3SiCF_3/CsF after 30 min measured at –80 ºC.

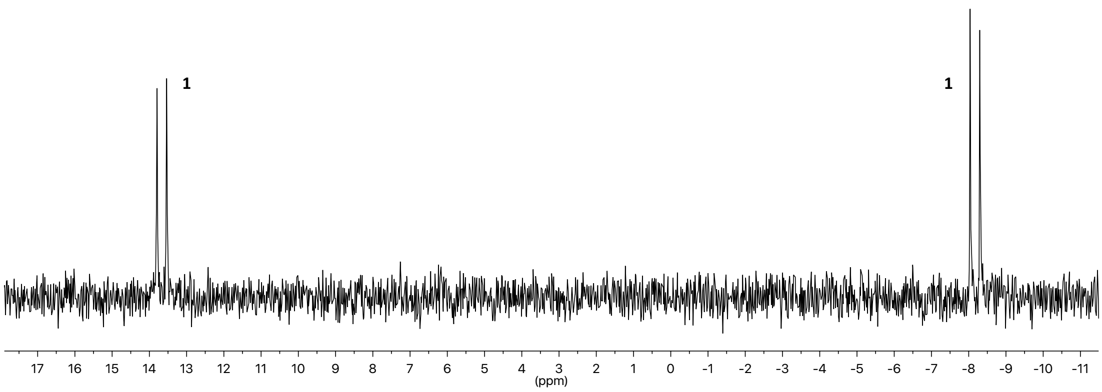
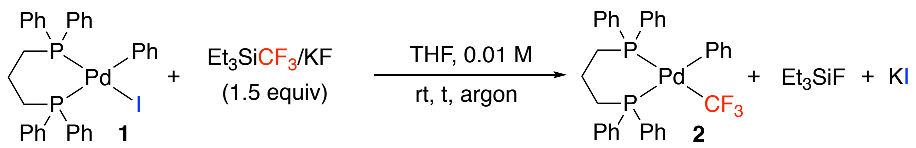


Figure S23. $^{31}P\{^1H\}$ NMR spectrum of the reaction of **1** and Et_3SiCF_3/CsF after 30 min measured at –80 ºC.

- **Transmetalation between complex 1 and Et_3SiCF_3/KF**



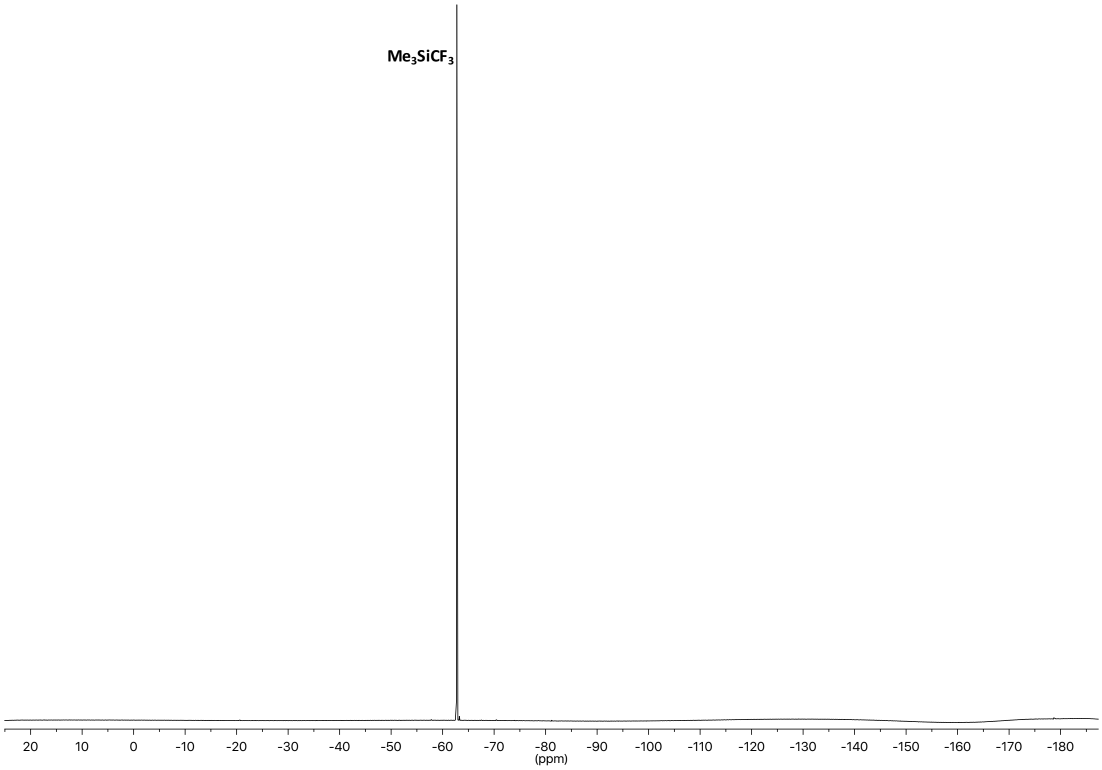


Figure S24. ^{19}F NMR spectrum of the reaction of **1** and Et_3SiCF_3/KF after 30 min measured at –80 ºC.

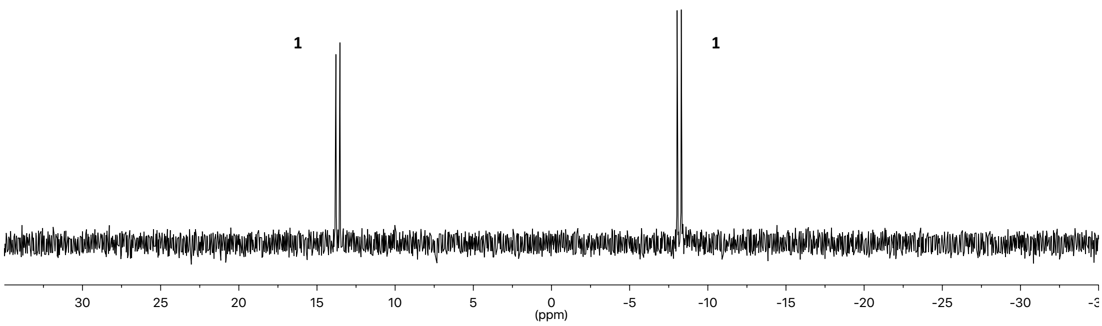
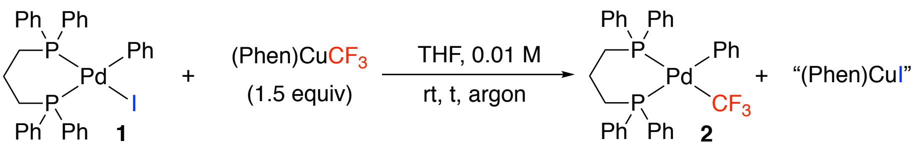


Figure S25. $^{31}P\{^1H\}$ NMR spectrum of the reaction of **1** and Et_3SiCF_3/KF after 30 min measured at –80 ºC.

- **Transmetalation between complex 1 and PhenCuCF$_3$**



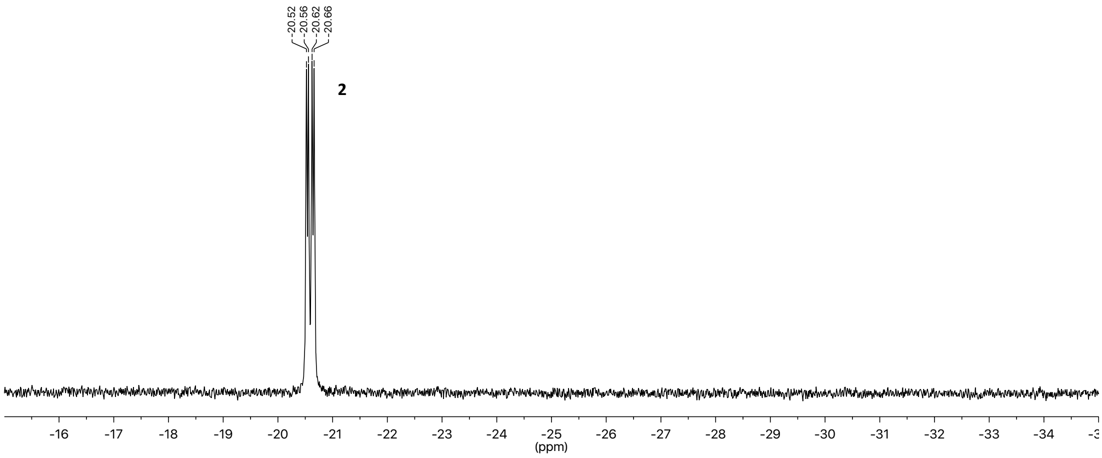


Figure S26. ^{19}F NMR spectrum of the reaction of **1** and PhenCuCF$_3$ after 10 min measured at –80 ºC. We only observe product **2** because the remaining copper species are insoluble in THF. For this reason, the same reaction was carried out during 16 h to see if any improvement of the yield was detected (see below).

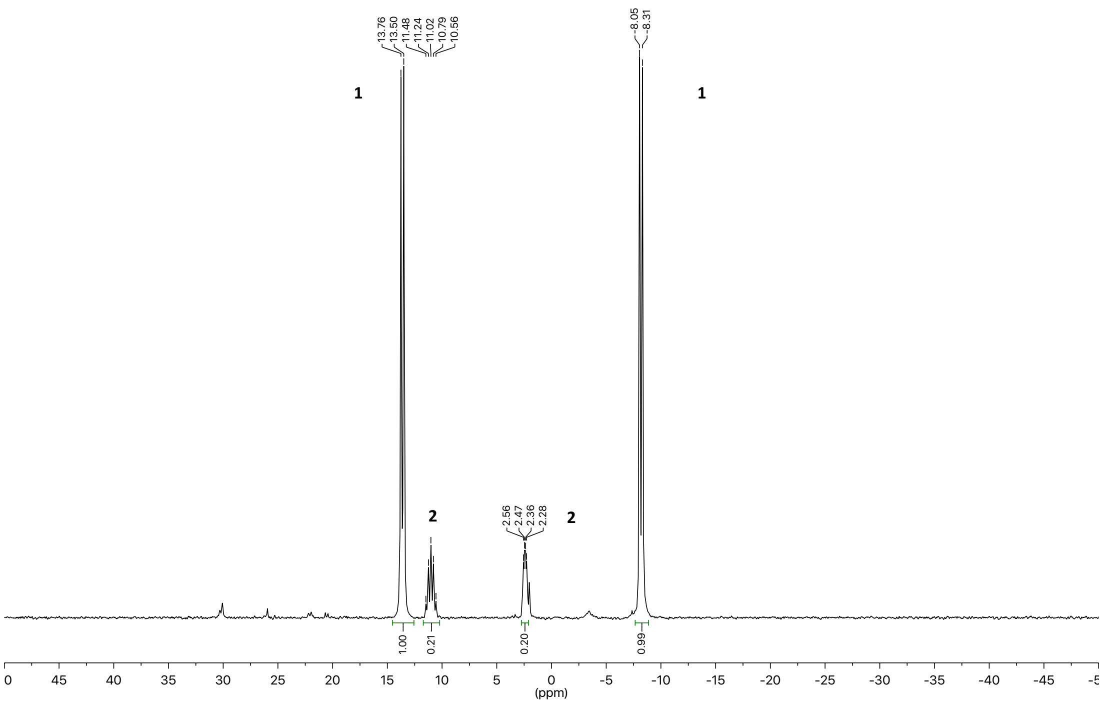


Figure S27. $^{31}P\{^{1}H\}$ NMR spectrum of the reaction of **1** and PhenCuCF$_3$ after 10 min measured at –80 ºC.

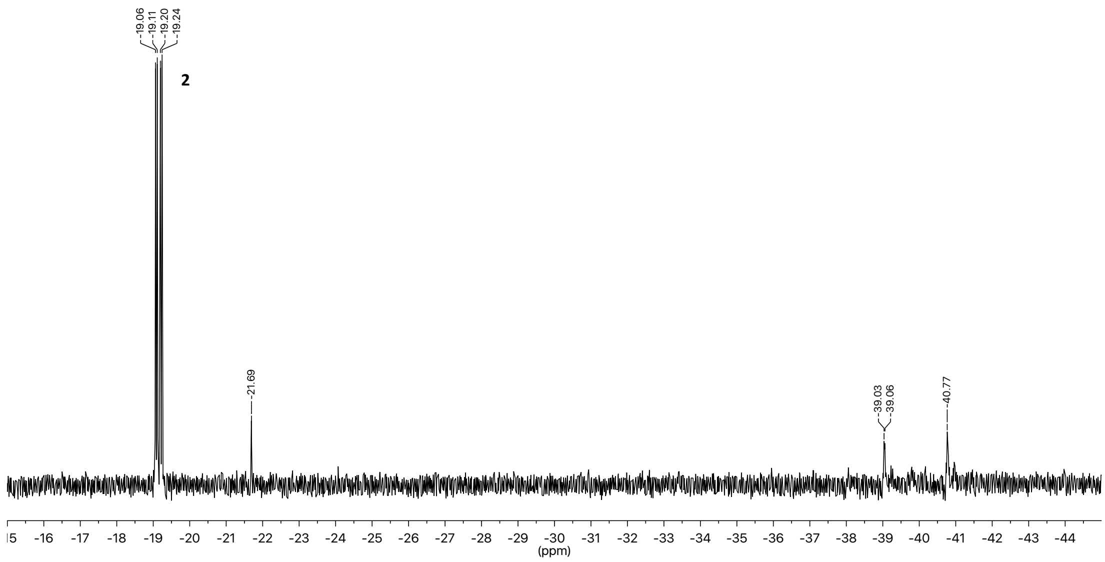


Figure S28. ^{19}F NMR spectrum of the reaction of **1** and $PhenCuCF_3$ at room temperature after 16 h of reaction.

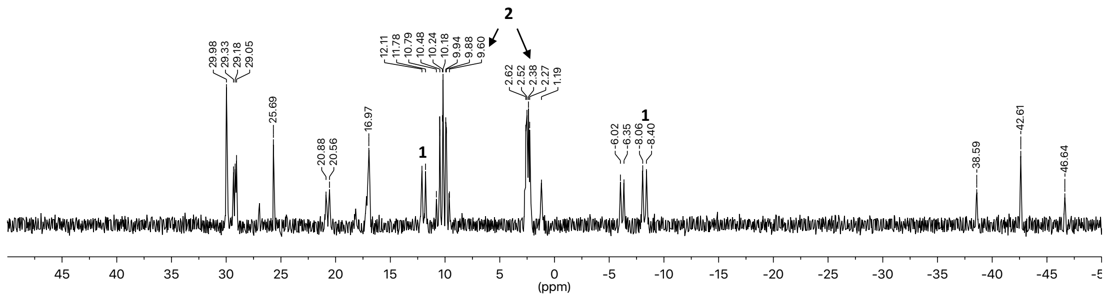
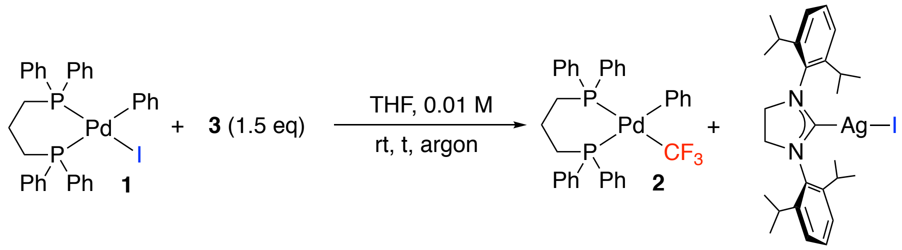


Figure S29. $^{31}P\{^1H\}$ NMR spectrum of the reaction of **1** and $PhenCuCF_3$ at room temperature after 16 h of reaction. The copper compound presents a limited behavior as CF_3-transfer reagent forming side products that limit the yield of the transformation.

- **Transmetalation between complexes 1 and 3**



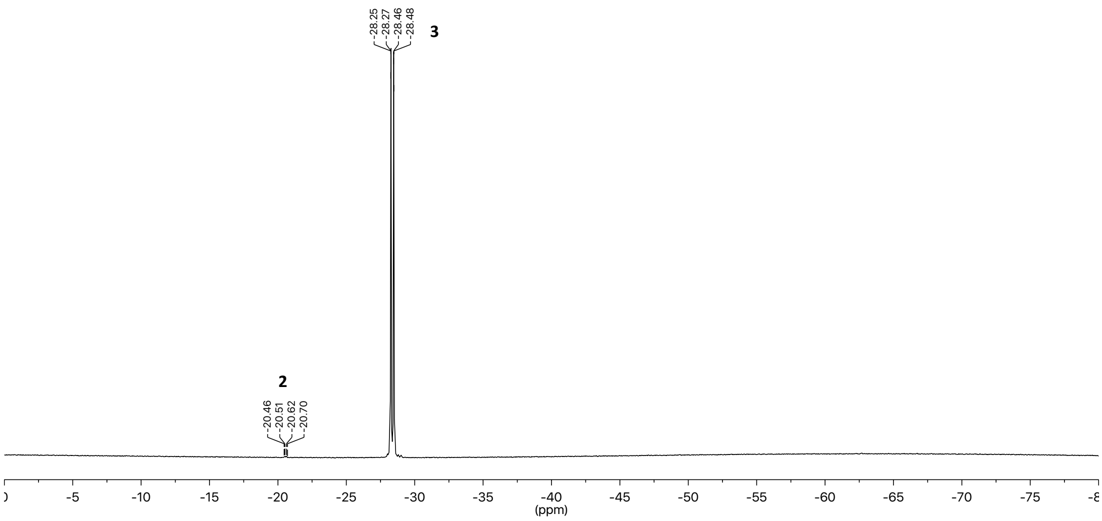


Figure S30. ^{19}F NMR spectrum of the reaction of **1** and **3** after 30 min measured at –80 ºC.

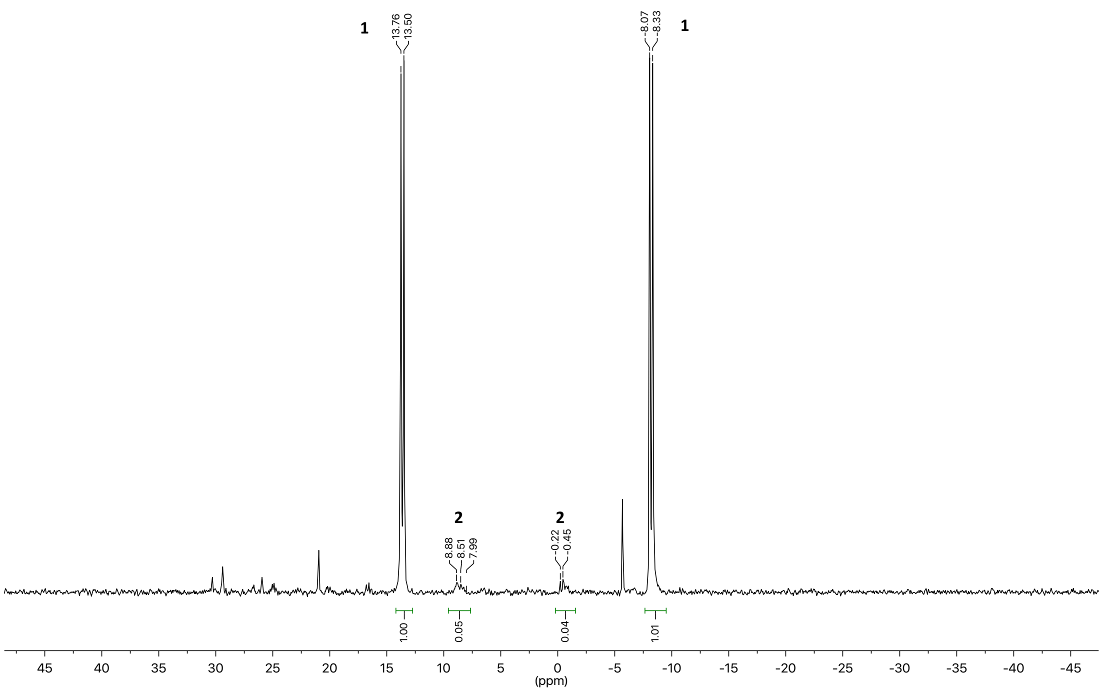
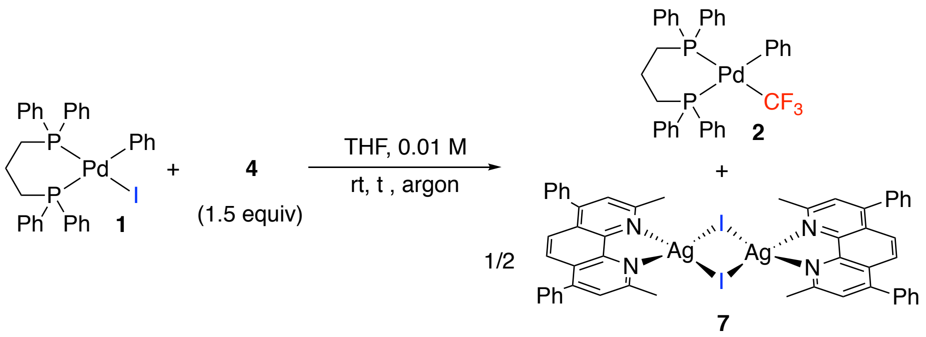


Figure S31. ^{31}P{^{1}H} NMR spectrum of the reaction of **1** and **3** after 30 min measured at –80 ºC.

- **Transmetalation between complexes 1 and 4**



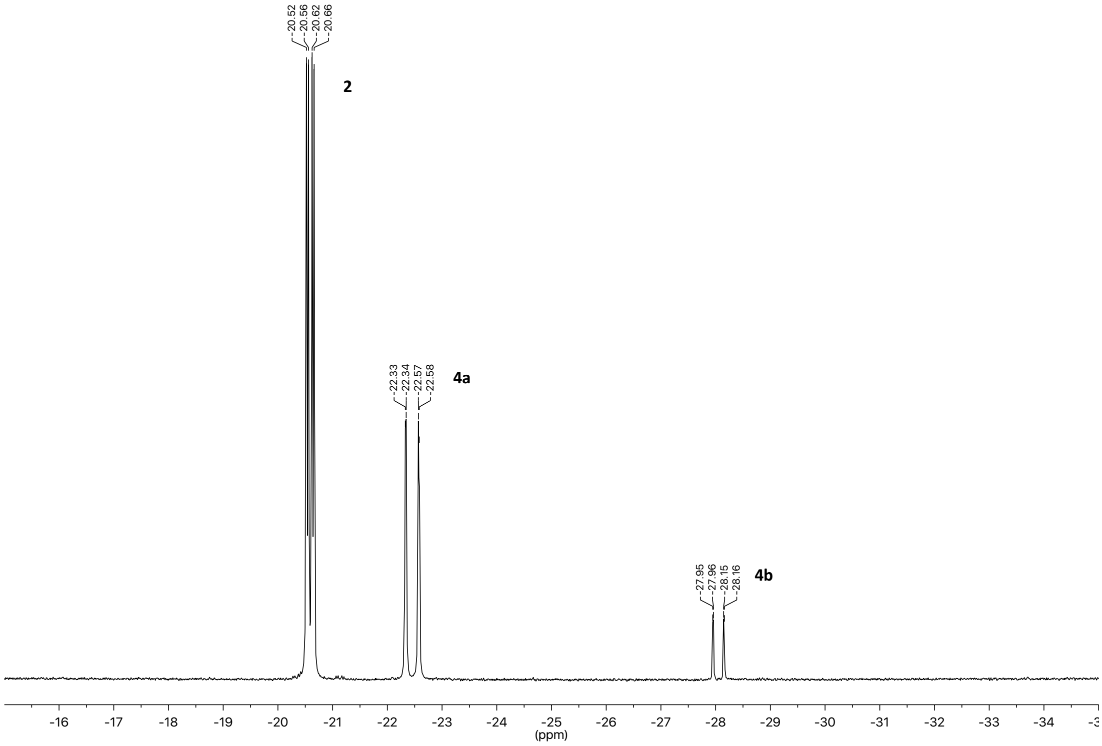


Figure S32. ^{19}F NMR spectrum of the reaction of **1** and **4** after 10 min measured at –80 ºC.

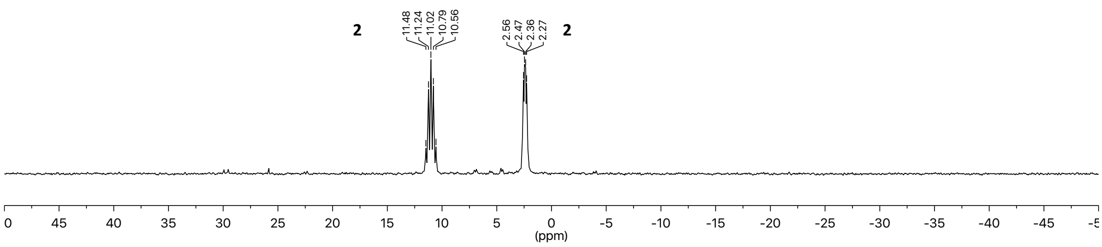
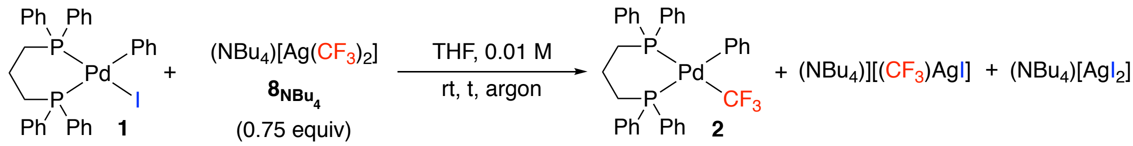


Figure S33. $^{31}P\{^{1}H\}$ NMR spectrum of the reaction of **1** and **4** after 10 min measured at –80 ºC.

- Transmetalation between complexes 1 and 8_{NBu_4}



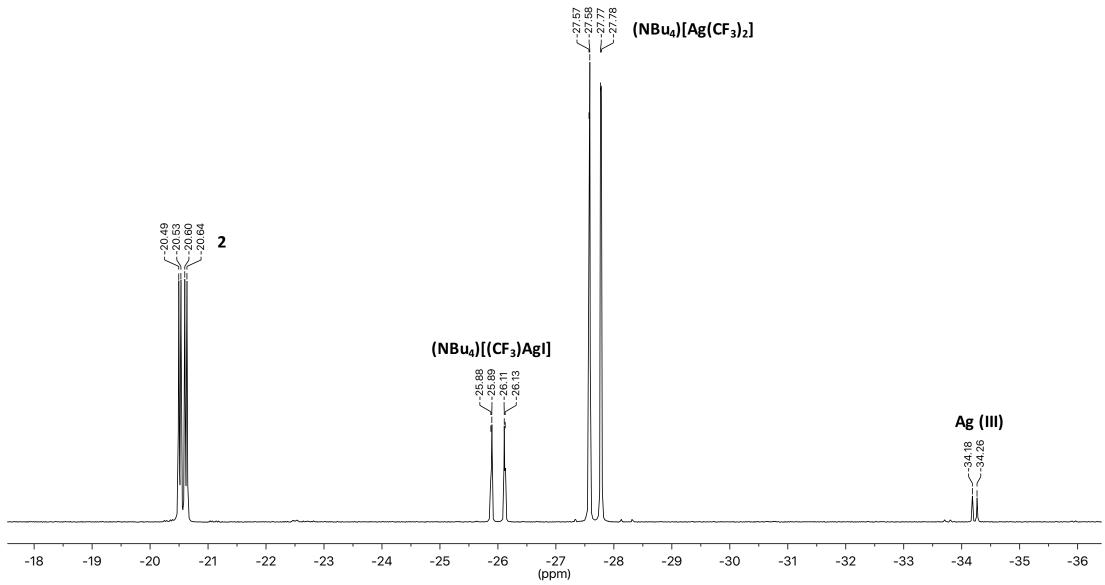


Figure S34. [19]F NMR spectrum of the reaction of **1** and $\mathbf{8_{NBu_4}}$ after 10 min measured at –80 ºC.

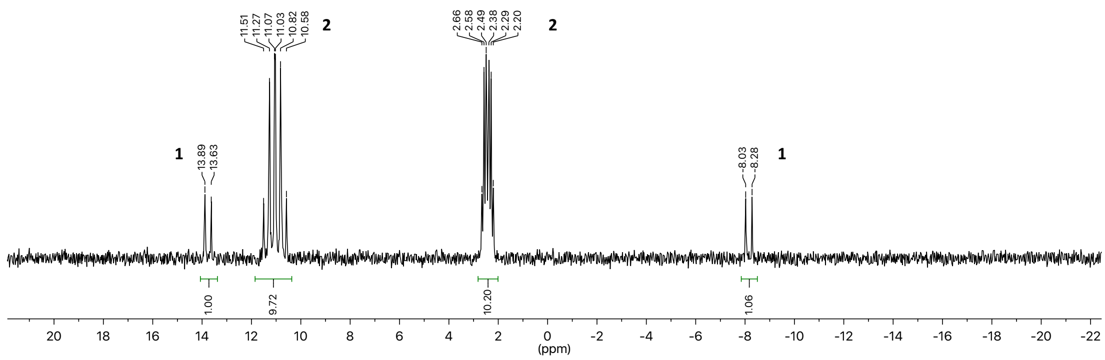
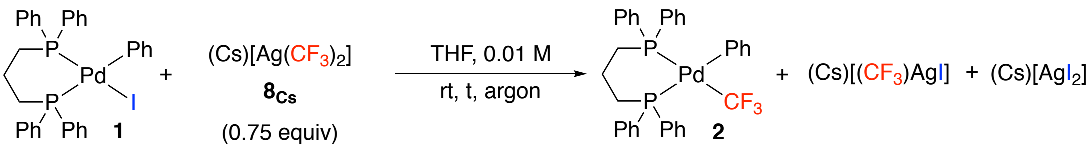


Figure S35. $^{31}P\{^1H\}$ NMR spectrum of the reaction of **1** and $\mathbf{8_{NBu_4}}$ after 10 min measured at –80 ºC.

- **Transmetalation between complexes 1 and 8_{Cs}**



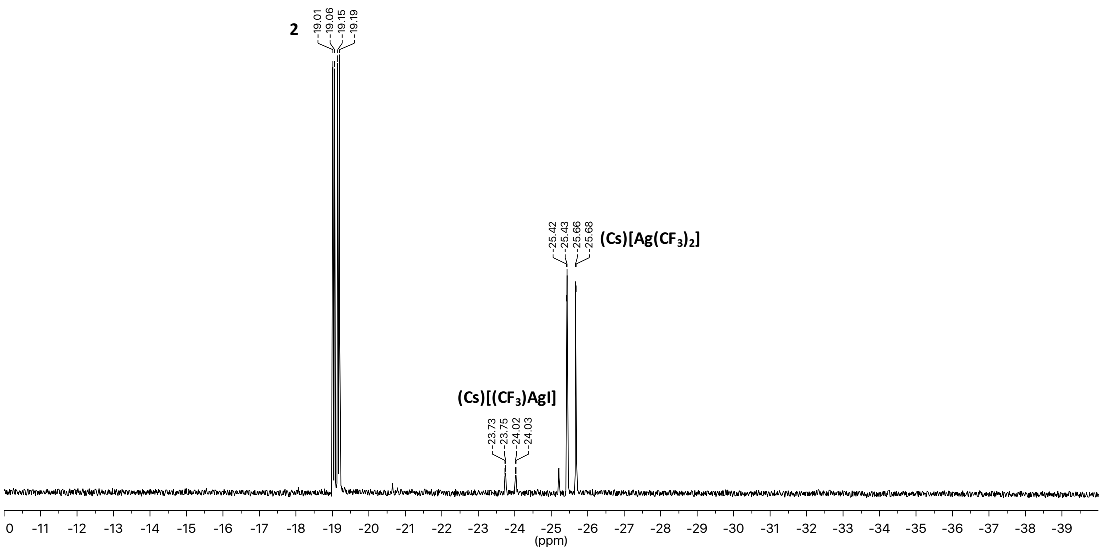


Figure S36. ^{19}F NMR spectrum of the reaction of **1** and **8_{Cs}** after 10 min measured at –80 ºC.

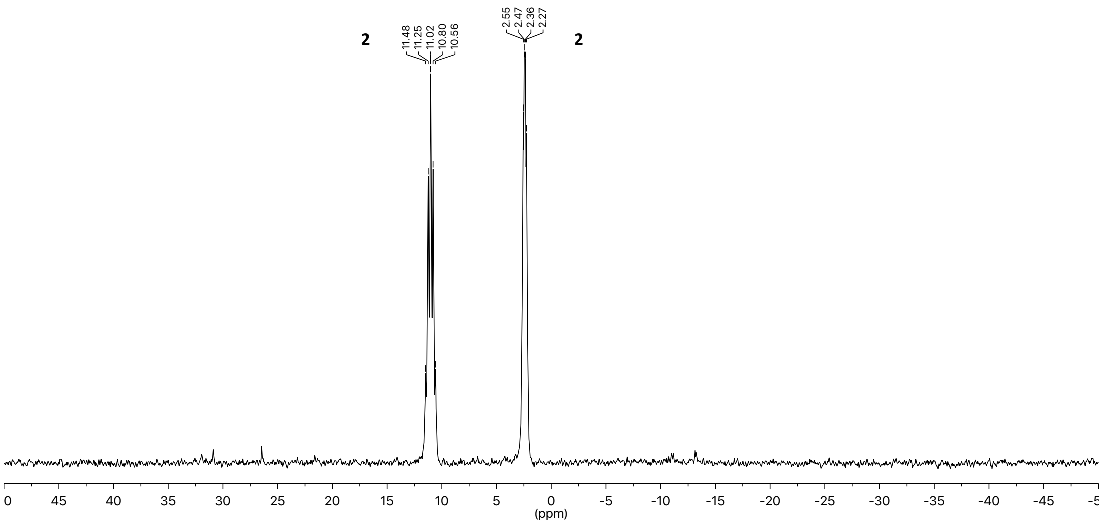
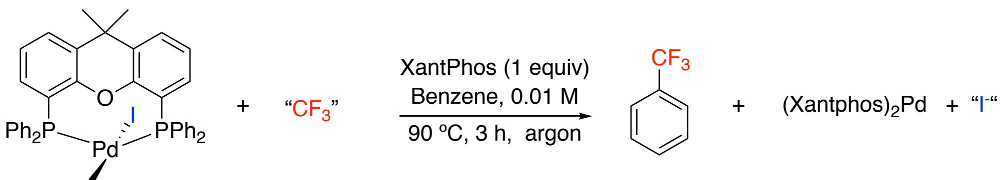


Figure S37. ^{31}P{^{1}H} NMR spectrum of the reaction of **1** and **8_{Cs}** after 10 min measured at –80 ºC.

Representative procedure for thermolysis of the mixture of (Xantphos)Pd(Ph)I (9) and different trifluoromethylating reagents

In a glovebox, a 5mL-crimped vial was charged with (Xantphos)Pd(Ph)I (**9**) (5.3 mg, 0.006 mmol), Xantphos (3.5 mg, 0.006 mmol) and the corresponding trifluoromethyl source [**4** (4.8 mg, 0.009 mmol), $\mathbf{8_{Cs}}$ (1.7 mg, 0.0045 mmol), $\mathbf{8_{NBu_4}}$ (2.2 mg, 0.0045 mmol)] or a combination of the fluoride source [CsF (3.6 mg, 0.024 mmol), KF (1.4 mg, 0.024 mmol), AgF (3.0 mg, 0.024 mmol), NBu_4F (24 μL of a 1 M solution in THF, 0.024 mmol)] with Me_3SiCF_3 or Et_3SiCF_3 (0.012 mmol, 100 μL of a 0.12 M stock solution in benzene). The reactions were dissolved in 0.6 mL of benzene (in case of MF/ R_3SiCF_3 only 0.5 mL of benzene were added) and heated at 90 ºC during 3 h. After that, each solution was filtered through a PTFE 13mm 0.2μm NSTR syringe filter and the internal standard was added; fluorobenzene (180 μL of a 0.06 M stock solution in cyclohexane) and/or 4,4´-difluorobiphenyl (250 μL of a 0.1 M stock solution in benzene). A ^{19}F NMR spectrum was acquired to determine the yield of benzotrifluoride and the different products obtained for the reaction. The experiments were performed at least duplicate. The yield was calculated taking the average of the different runs and it was determined by comparing the original mass of the sample **9** (limiting reactive) to its number of moles against the internal standard.



9   11

Table S8. % yield of $PhCF_3$ using different CF_3 sources

Entry	CF_3 Source	Equiv	11 (%)
1	**4**	1.5	70
2	$\mathbf{8_{NBu_4}}$	0.75	42
3	$\mathbf{8_{Cs}}$	0.75	84
4	Me_3SiCF_3/CsF	2/4	14
5	Me_3SiCF_3/KF	2/4	0
6	Me_3SiCF_3/AgF	2/4	9
7	Me_3SiCF_3/NBu_4F	2/4	4
8	Et_3SiCF_3/CsF	2/4	20
9	Et_3SiCF_3/KF	2/4	0

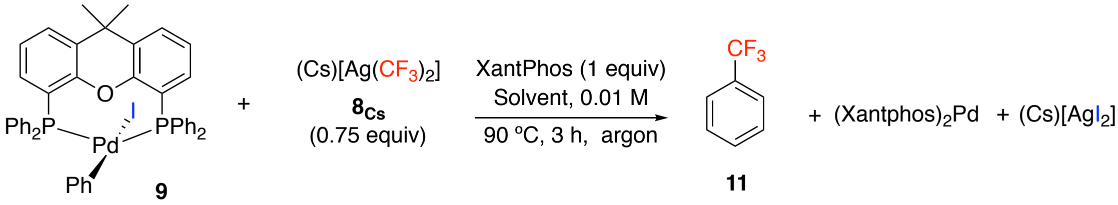


Table S9. % yield of $PhCF_3$ using **8$_{Cs}$** under different conditions

Entry	Solvent	Deviation from standard conditions	11 (%)
1	THF	-	36
2	Benzene	-	84
3	Benzene	1h, 90 °C	69
4	Benzene	Without Xantphos	42
5	Benzene	Without Pd complex	-
6*	Benzene	Without Xantphos and Pd complex	-
7*	Toluene	Without Xantphos and Pd complex	-

* The complex **8$_{Cs}$** decomposes in benzene and toluene (0.01 M or 0.002 M) after 15 min at room temperature or 95 °C while stirring at 1200 rpm. After these reactions, a transparent solution and a black solid that presumably corresponds to silver metallic were observed. The transparent solution was analyzed by ^{19}F NMR and only HCF_3 was observed.

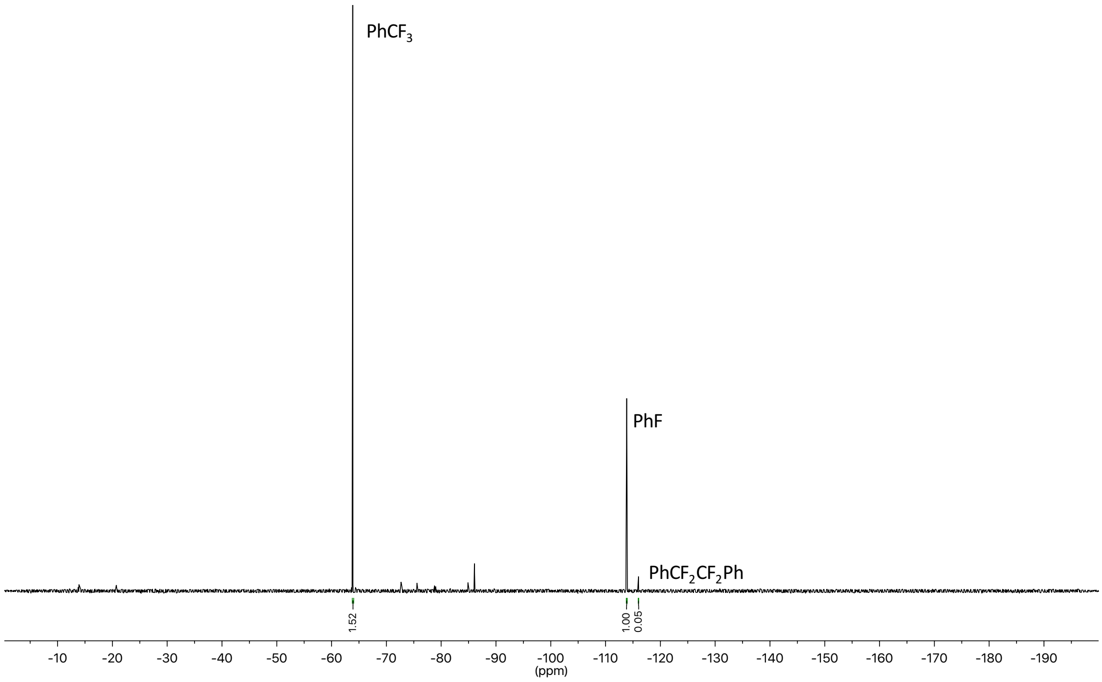


Figure S38. ^{19}F NMR spectrum of the reaction mixture after heating at 90 °C during 3 h using **8$_{Cs}$**. We observe the formation of a 3% of $PhCF_2CF_2Ph$ as by-product.

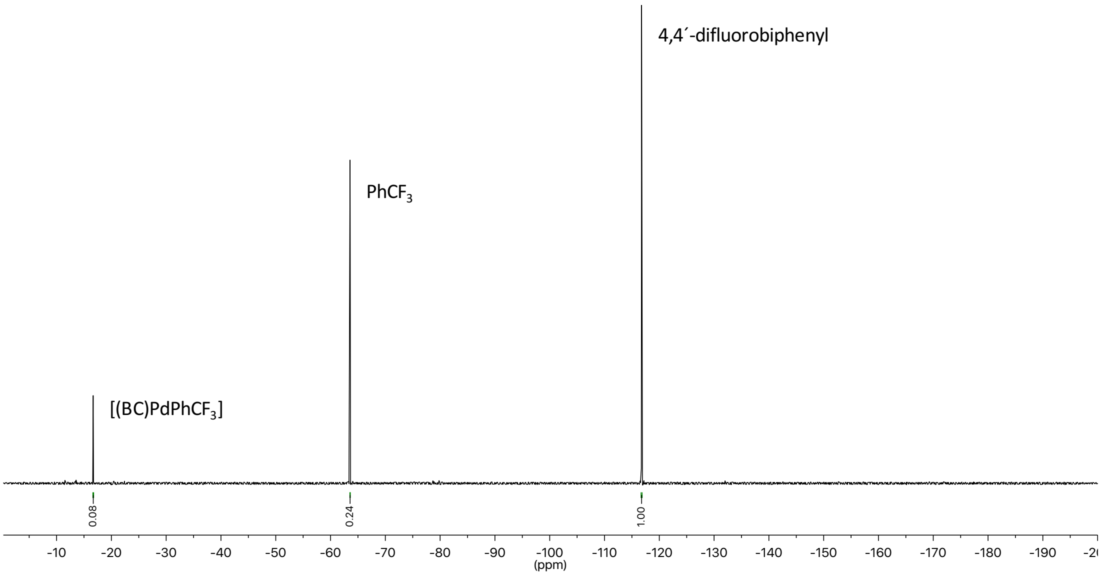


Figure S39. [19]F NMR spectrum of the reaction mixture after heating at 90 ºC during 3 h using **4**. The other [19]F signal (δ −16.68 ppm) is related to the formation of the (Bc)Pd(Ph)(CF_3) (unconfirmed, but a reasonable assumption based on the chemical shift of related species).[4,15]

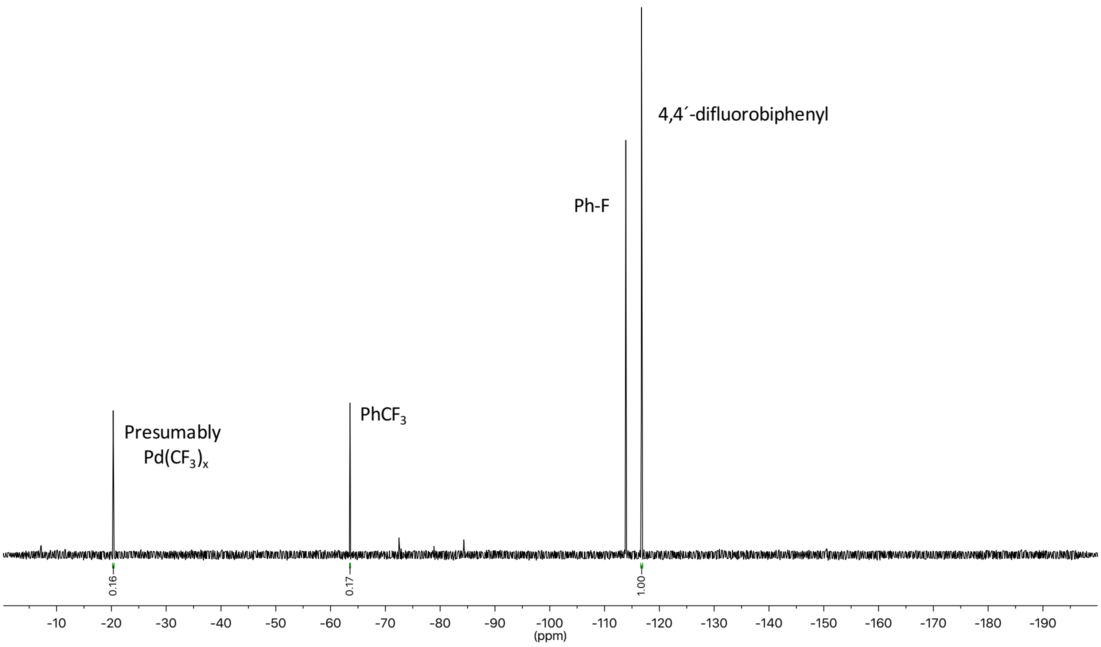


Figure S40. [19]F NMR spectrum of the reaction mixture after heating at 90 ºC during 3 h using **8_{NBu_4}**.

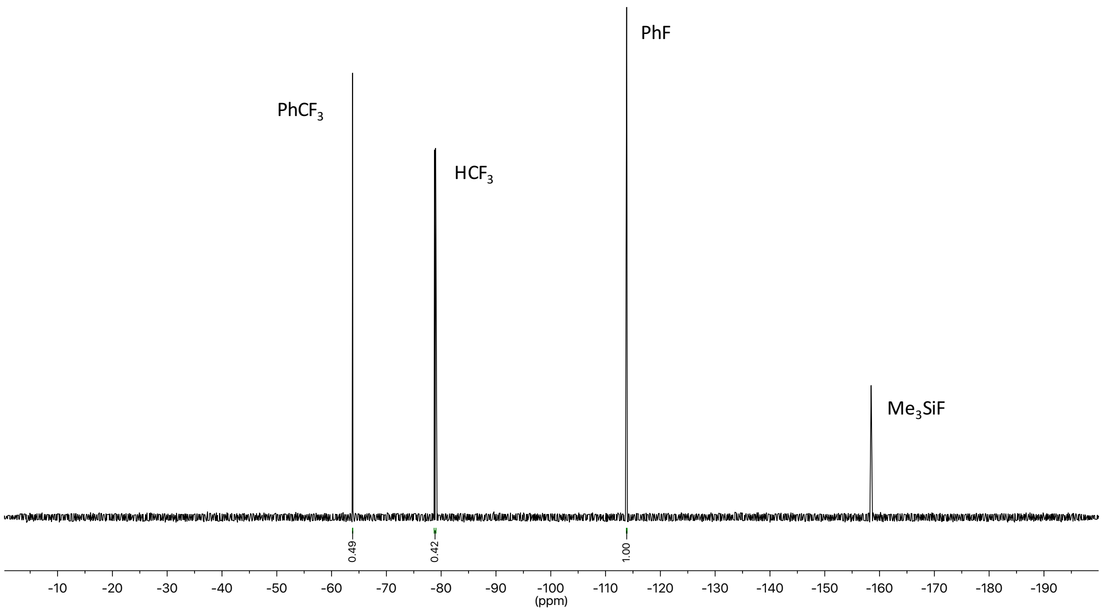


Figure S41. ^{19}F NMR spectrum of the reaction mixture after heating at 90 ºC during 3 h using Me_3SiCF_3/CsF.

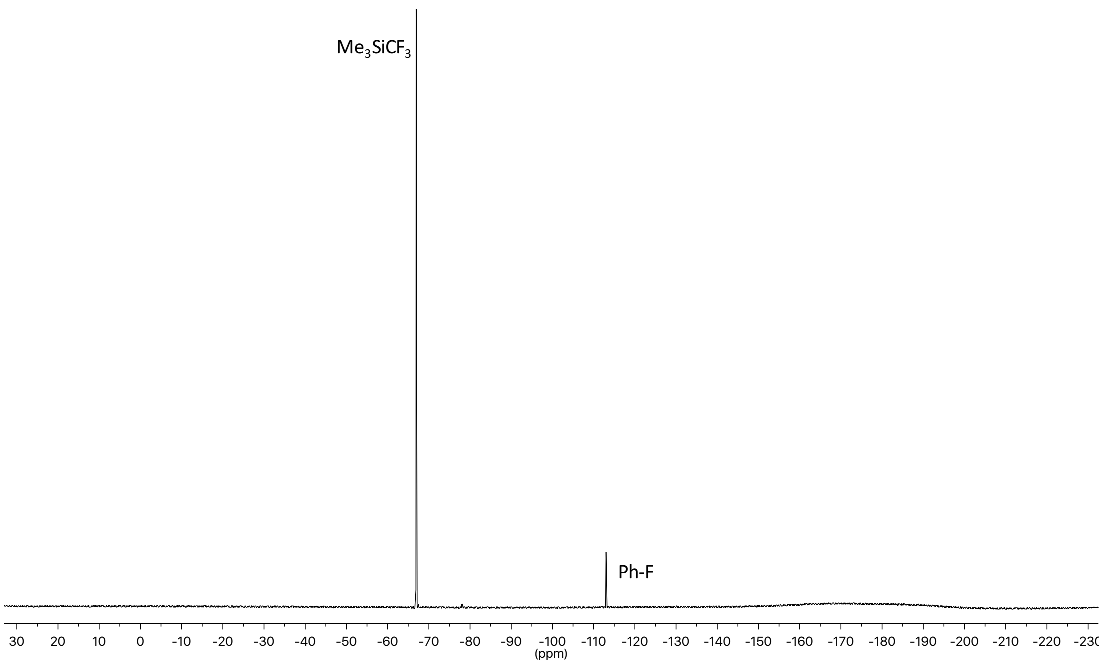


Figure S42. ^{19}F NMR spectrum of the reaction mixture after heating at 90 ºC during 3 h using Me_3SiCF_3/KF.

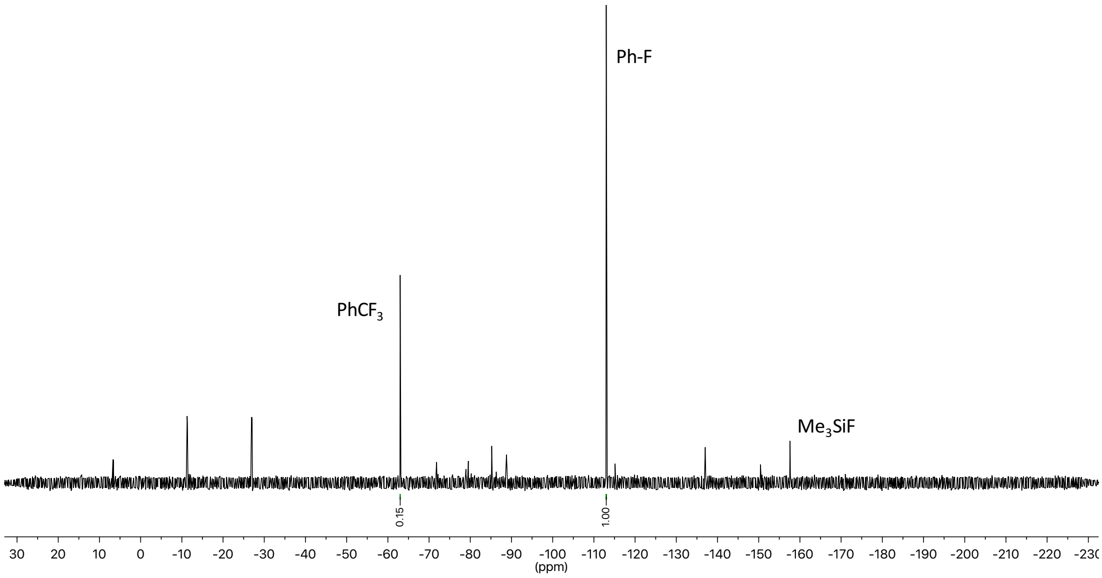


Figure S43. [19]F NMR spectrum of the reaction mixture after heating at 90 ºC during 3 h using Me_3SiCF_3/AgF.

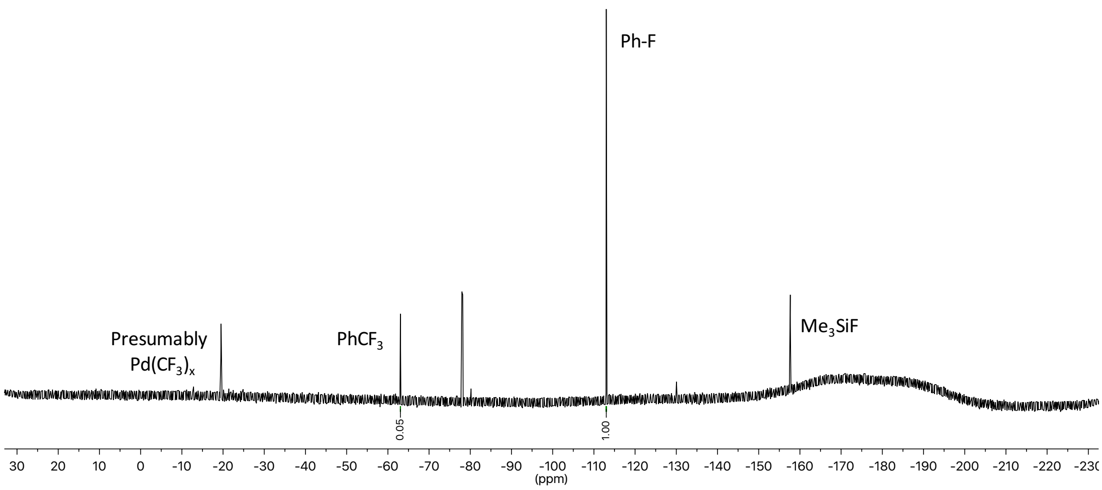


Figure S44. [19]F NMR spectrum of the reaction mixture after heating at 90 ºC during 3 h using Me_3SiCF_3/NBu_4F.

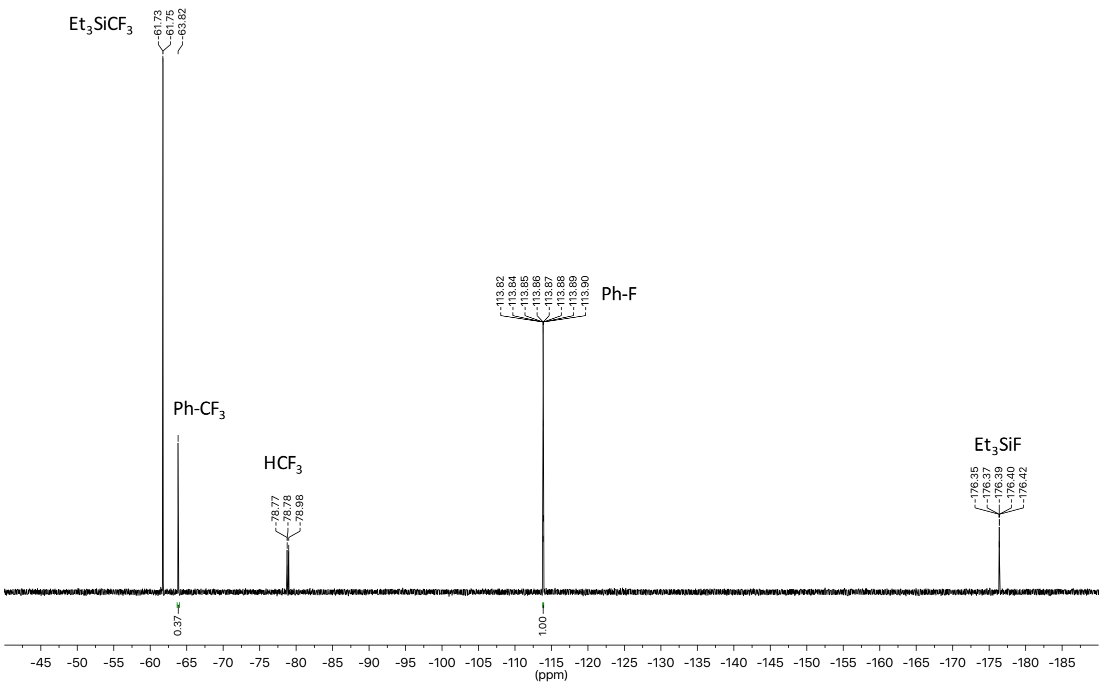


Figure S45. ^{19}F NMR spectrum of the reaction mixture after heating at 90 ºC during 3 h using Et_3SiCF_3/CsF.

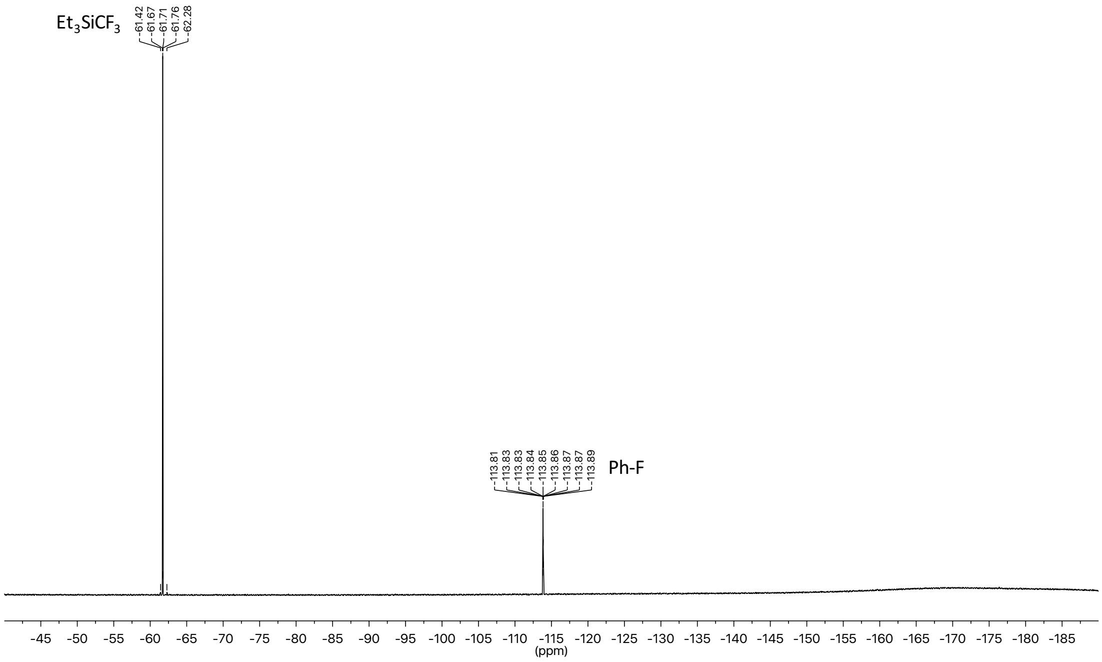


Figure S46. ^{19}F NMR spectrum of the reaction mixture after heating at 90 ºC during 3 h using Et_3SiCF_3/KF.

Grushin reported that (Xantphos)Pd(Ph)(CF_3) (**10**) could not be prepared using complex (Xantphos)Pd(Ph)I (**9**) and Me_3SiCF_3/F^- due to the facile and irreversible displacement of Xantphos by CF_3^- that is uncontrollably released from Me_3SiCF_3/F^-.[16] Indeed, it was proposed that the displacement of the Xantphos ligand would give inactive poly(trifluoromethyl) complexes $(L_m)Pd(CF_3)_x(Ar)$.[16,17]

In our case, we only observe the presumably formation of these complexes (δ ≈ –20 ppm) in the reaction of (Xantphos)Pd(Ph)I (**9**) using $(NBu_4)[Ag(CF_3)_2]$ (**8_{NBu_4}**) or the mixture of Me_3SiCF_3/NBu_4F.

In an attempt to gain insight into the reaction between (Xantphos)Pd(Ph)I (**9**) and Me_3SiCF_3/F^- (Table S8, Entry 4), diverse reactions were carried out changing different parameters.

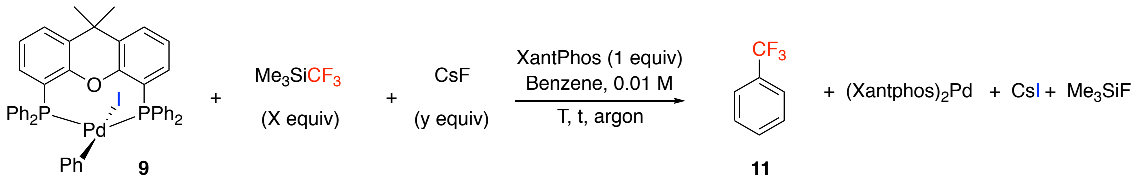


Table S10. % yield of $PhCF_3$ using Me_3SiCF_3/CsF in different conditions

Entry	Equiv Me_3SiCF_3/CsF	Time (h)	Temperature (ºC)	11 (%)
1	2/4	3	25	0
2	2/4	3	90	14
3	2/4	6	90	12
4	4/4	6	90	20

These results suggest that the time of the reaction is not critical for the yield of $PhCF_3$ based on entries 2 and 3.

Interestingly, for entry 4, ^{19}F and ^{31}P NMR experiments showed that all the starting materials and the product $(Xantphos)Pd(Ph)(CF_3)$ (**10**) resulting from the transmetalation have been fully consumed. We hypothesized that the reasons that limit the yield of the transformation are the poor selectivity of the reaction and/or the decomposition of Me_3SiCF_3.

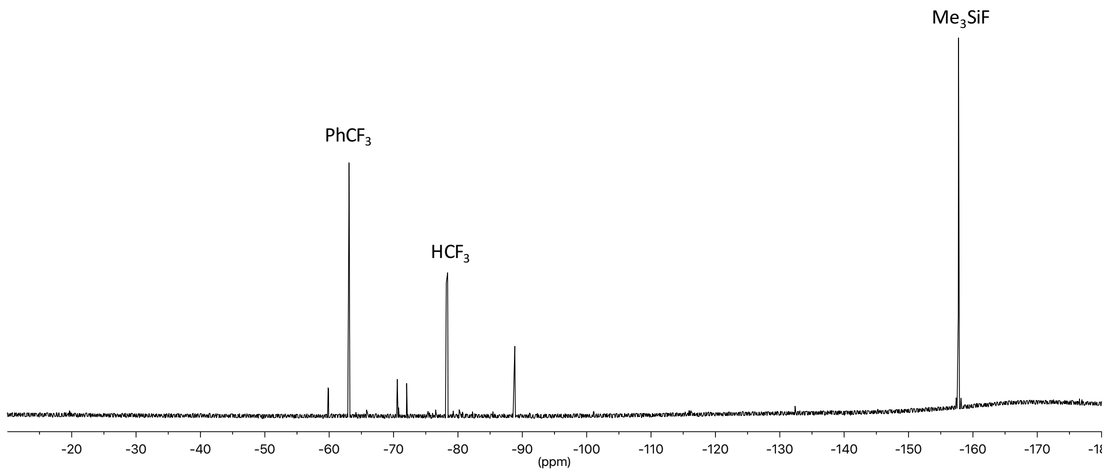


Figure S47. ^{19}F NMR spectrum of the reaction mixture after heating at 90 ºC during 6 h using 4 equiv of Me_3SiCF_3 and 4 equiv of CsF.

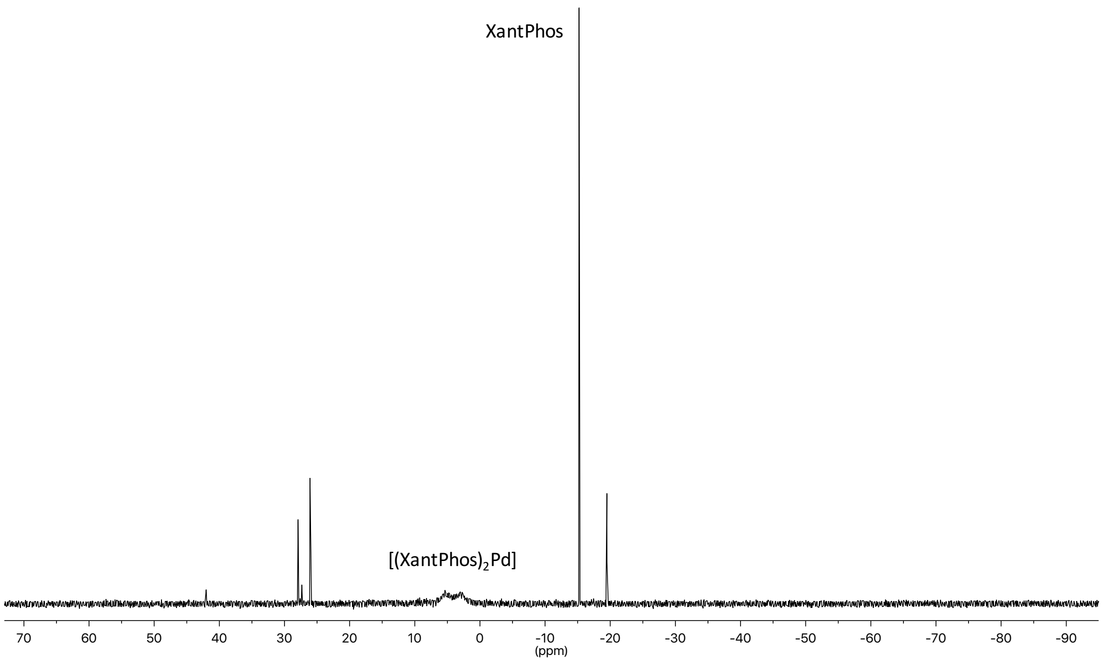
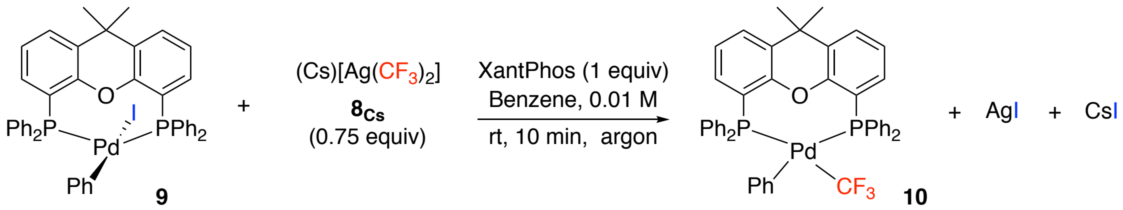


Figure S48. $^{31}P\{^1H\}$ NMR spectrum of the reaction mixture after heating at 90 ºC during 6 h using 4 equiv of Me_3SiCF_3 and 4 eq of CsF.

Direct proof of the intermediation of (Xantphos)Pd(Ph)(CF_3) (10) complex in the reductive elimination process

In a glovebox, a 5mL-crimped vial was charged with (Xantphos)Pd(Ph)I (**9**) (5.3 mg, 0.006 mmol), Xantphos (3.5 mg, 0.006 mmol) and (Cs)[Ag(CF_3)$_2$] (**8$_{Cs}$**) (1.7 mg, 0.0045 mmol), dissolved in benzene (0.6 mL) and stirred at room temperature during 10 min. After that, the bright yellow solution was transferred to a NMR tube and the solvent was evaporated. Next, 0.6 mL of toluene were added and ^{19}F NMR (ns = 64 scans) and ^{31}P NMR (ns = 1024 scans) spectra were measured at –50 ºC.
The same reaction was repeated using Me_3SiCF_3/CsF and no (Xantphos)Pd(Ph)(CF_3) complex (**10**) was observed.



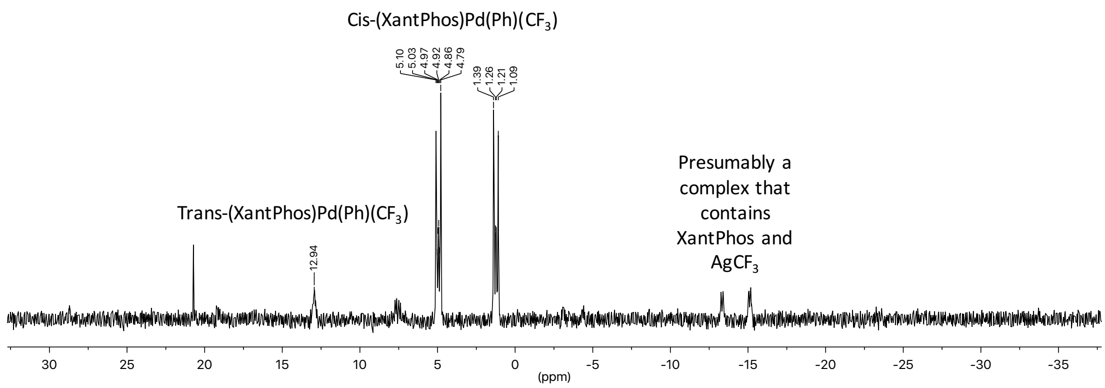


Figure S49. ^{31}P{^{1}H} NMR spectrum after 10 min of reaction in benzene measured at –50 ºC.

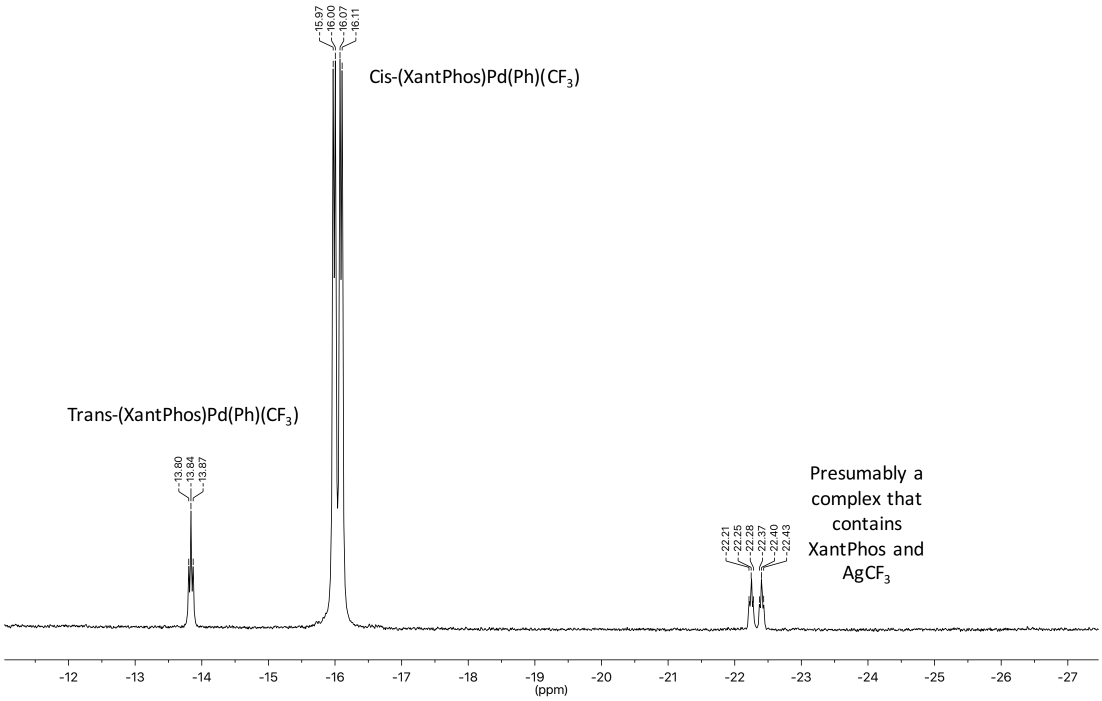
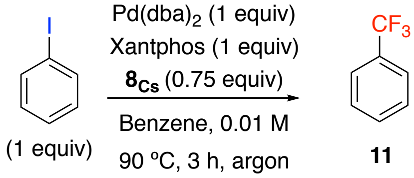


Figure S50. ^{19}F NMR spectrum after 10 min of reaction in benzene measured at –50 ºC. The spectrum was recorded between 100 and –500 ppm and no other signals were observed discarding the participation of Pd(IV) species. The same signal at –22.4 ppm appears by mixing (Cs)[Ag(CF$_3$)$_2$] (**8$_{Cs}$**) and Xantphos in the same reaction conditions.

Competency of (Cs)[Ag(CF_3)$_2$] (8_{Cs}) as CF_3 source under relevant stoichiometric conditions

As mentioned in the main text, a slow nucleophilic trifluoromethylation leads to undesired reactions by "mismatched" group exchanges. The enhanced ability of trifluoromethyl Pd aryls to undergo transmetalation with other aryl Pd complexes, including (Xantphos)Pd(Ar)I, results in the formation of the catalytically inactive (Xantphos)Pd(CF_3)I and (Xantphos)Pd(Ar)$_2$ that undergoes Ar–Ar reductive elimination. This transmetalation path is favored by high concentrations and temperature. To test the effectiveness of **8_{Cs}** as new transmetalating reagent different experiments were carried out.



In a glovebox, a 5mL-crimped vial containing a 12mmx3mm PTFE cylindrical stirrer was charged with Pd(dba)$_2$ (3.4 mg, 0.006 mmol), Xantphos (3.5 mg, 0.006 mmol) and **8_{Cs}** (1.7 mg, 0.0045 mmol). The reaction was dissolved in 0.6 mL of benzene and PhI was added (10 µL of a 0.6 M stock solution in toluene, 0.006 mmol). The suspension was taken out of the glovebox and the mixture was heated at 90 ºC and stirred at 1200 rpm during 3 h. After that, the solution was filtered through a PTFE 13mm 0.2µm NSTR syringe filter and the internal standard was added; fluorobenzene (180 µL of a 0.06 M stock solution in cyclohexane). A ^{19}F NMR spectrum was acquired to determine the yield of benzotrifluoride and the different products obtained for the reaction. The yield was determined by comparing the original mass of Pd(dba)$_2$ (limiting reactive) to its number of moles against the internal standard. The reaction afforded a 57% of benzotrifluoride and a 10% of the catalytically inactive (Xantphos)Pd(CF_3)I. This result suggests that lower concentrations of Pd are needed to slow down the undesired transmetalation that is a bimolecular reaction.

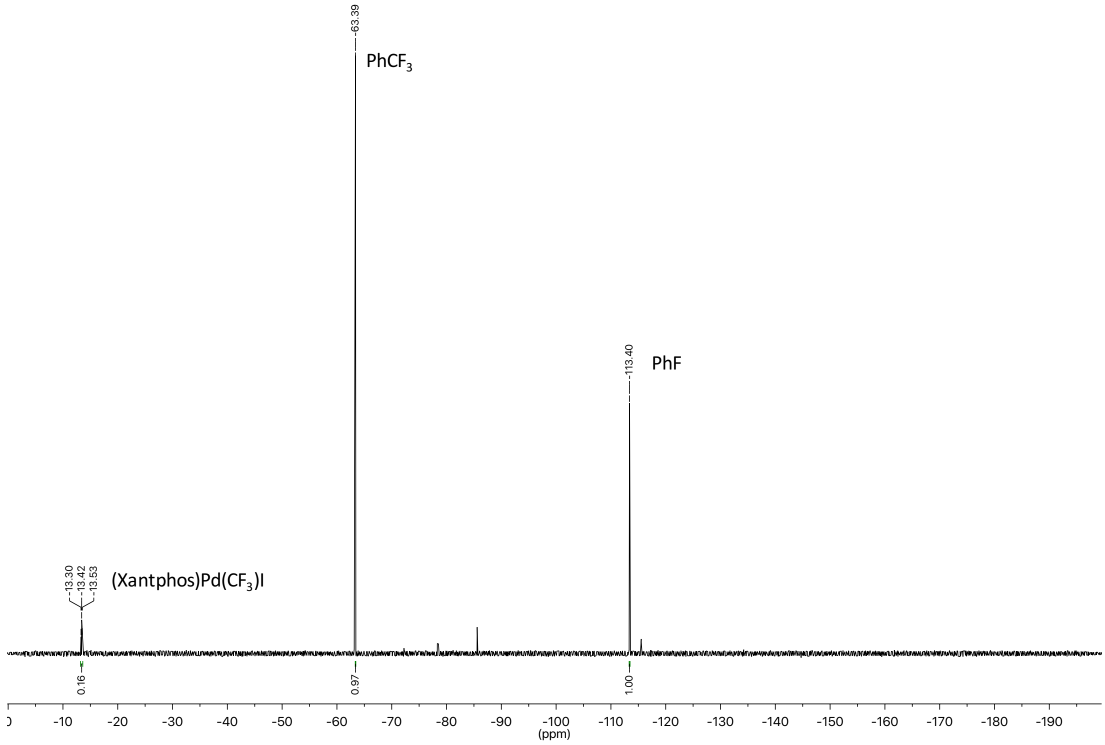


Figure S51. ^{19}F NMR spectrum of the reaction mixture after heating at 90 ºC during 3 h.

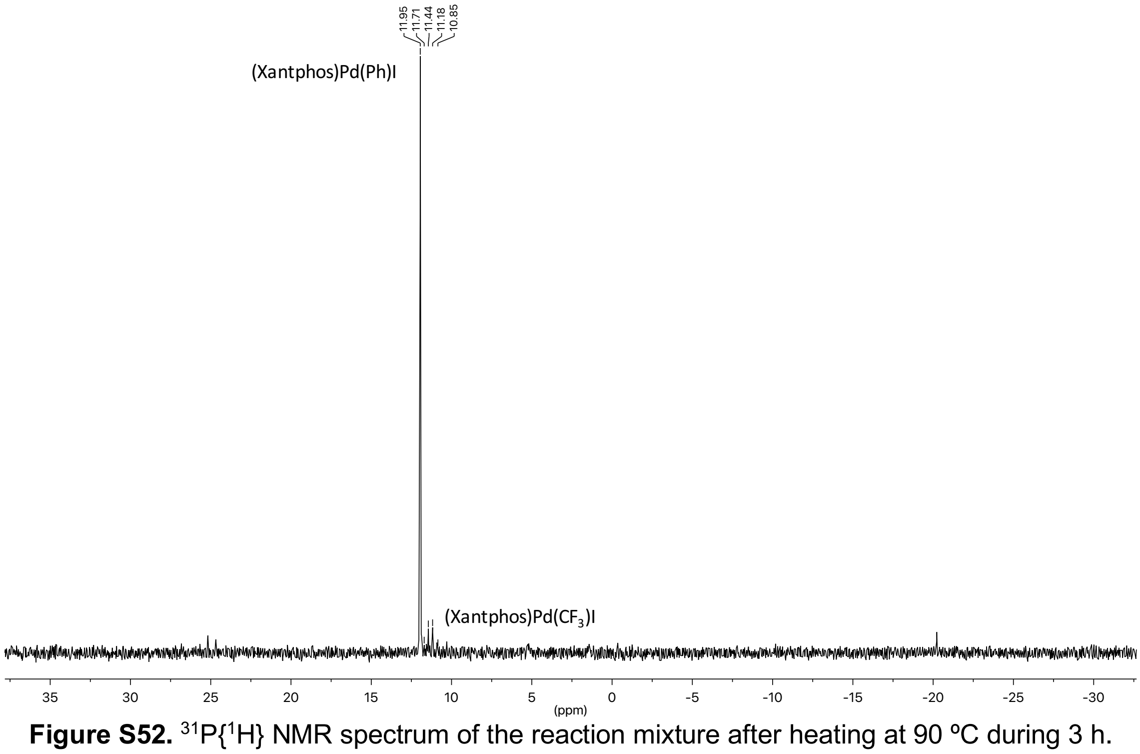
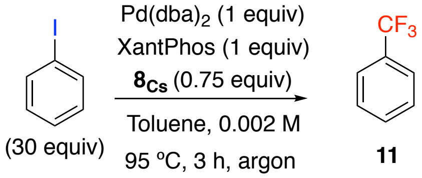


Figure S52. ^{31}P{^{1}H} NMR spectrum of the reaction mixture after heating at 90 ºC during 3 h.

After some screening of solvent, temperature and concentration, the best conditions were developed, showing the compatibility of all the different steps and **8$_{Cs}$** in the Pd-mediated trifluoromethylation of phenyl iodide.



In a glovebox, a 5mL-crimped vial containing a 12mmx3mm PTFE cylindrical stirrer was charged with $Pd(dba)_2$ (3.4 mg, 0.006 mmol), Xantphos (3.5 mg, 0.006 mmol) and **8**$_{\mathbf{Cs}}$ (1.7 mg, 0.0045 mmol). The reaction was dissolved in 3 mL of toluene and PhI was added (30 μL, 0.18 mmol). The suspension was taken out of the glovebox and the mixture was heated at 95 ºC and stirred at 1200 rpm during 3 h. After that, the solution was filtered through a PTFE 13mm 0.2μm NSTR syringe filter and an aliquot of 1 mL was added to a NMR tube together with the internal standard; fluorobenzene (100 μL of a 0.06 M stock solution in cyclohexane). A ^{19}F NMR spectrum was acquired to determine the yield of benzotrifluoride and the different products obtained for the reaction. The experiment was performed in duplicate. The yield was calculated taking the average of the different runs and it was determined by comparing the original mass of $Pd(dba)_2$ (limiting reactive) to its number of moles against the internal standard. Since the stability of **8**$_{\mathbf{Cs}}$ is limited in toluene at 95 ºC (pS71) and the proof that $(Cs)[(CF_3)AgI]$ is capable of transferring the CF_3 group (see reference 20 in the main text), we can discard a second turn in the cycle.

The reaction afforded a 91% of benzotrifluoride (**11**) and no catalytically inactive $(Xantphos)Pd(CF_3)I$. $^{31}P\{^1H\}$ NMR experiment shows mainly the oxidative addition product (Xantphos)Pd(Ph)I. This result clearly demonstrates the compatibility of **8**$_{\mathbf{Cs}}$ as a CF_3 source in the Pd-mediated trifluoromethylation reactions. A fine tuning of the reaction conditions and a fast nucleophilic trifluoromethylation reagent **8**$_{\mathbf{Cs}}$ do not lead to mismatched group exchanges, a sink for Pd in catalysis.

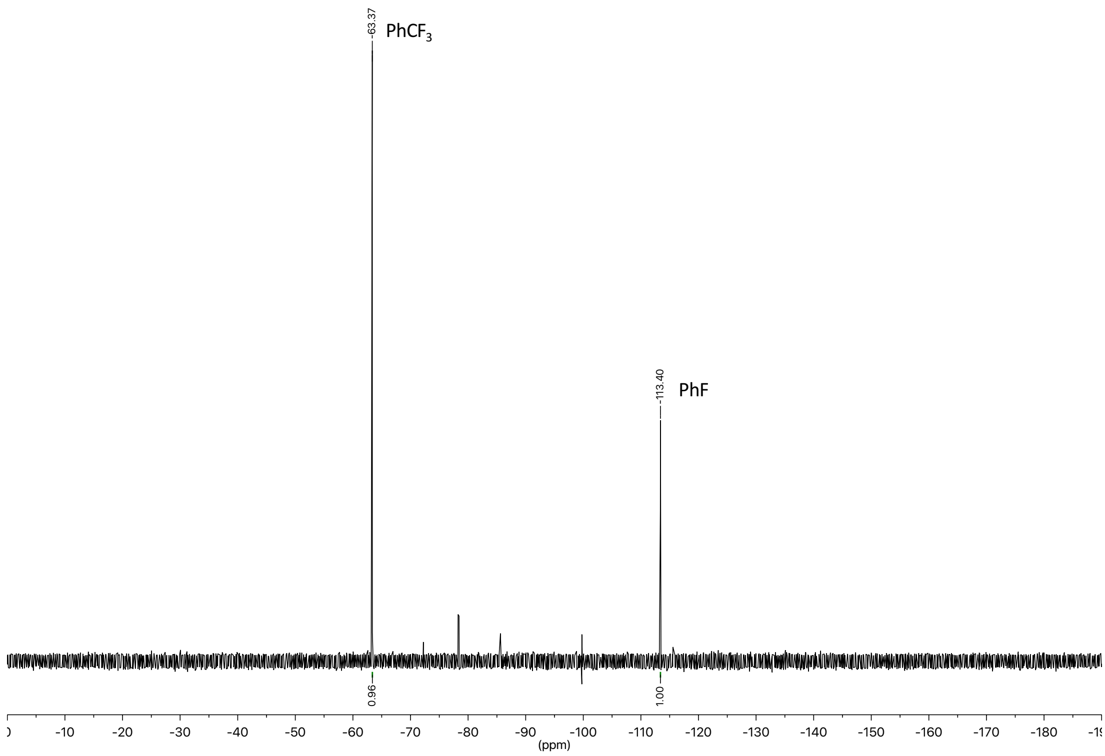


Figure S53. ^{19}F NMR spectrum of the reaction mixture after heating at 95 ºC during 3 h.

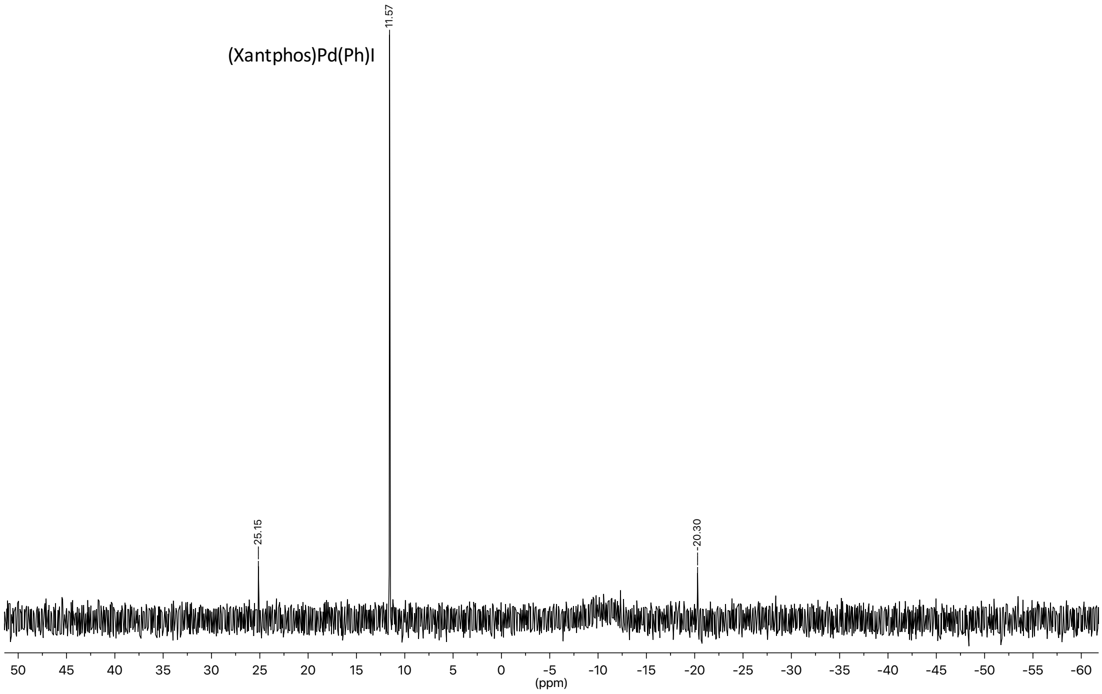


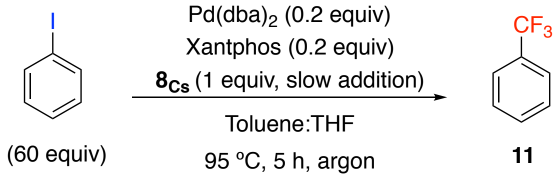
Figure S54. $^{31}P\{^{1}H\}$ NMR spectrum of the reaction mixture after heating at 95 ºC during 3 h.

Competency and challenges of (Cs)[Ag(CF_3)$_2$] (**8$_{Cs}$**) as CF_3 source in Pd-catalyzed trifluoromethylation reactions

Obviously, catalytic conditions are quite different than the stoichiometric ones and diverse parameters have to be taken into account.

- The suitability of **8$_{Cs}$** in solution is limited by the temperatures needed for the reductive elimination process (80-100 ºC). The decomposition of complex **8$_{Cs}$** in solution at these temperatures takes place in 15 min (see pS72).
- Complex **8$_{Cs}$** is only completely soluble in THF and DMF, where the reductive elimination is much more inefficient.
- Potential secondary reactions between Xantphos and complex **8$_{Cs}$**, specially in polar solvents.

All of these challenges can be partially circumvented adding slowly complex **8$_{Cs}$** during the time of the reaction.



In a glovebox, a schlenk with a female joint ST/NS 29/32, a height of 19 cm and a diameter of 28 cm containing a 12mmx3mm PTFE cylindrical stirrer was charged with Pd(dba)$_2$ (1.8 mg, 0.003 mmol) and Xantphos (1.8 mg, 0.003 mmol) and covered with a septum of 30.7 mm. The solids were dissolved in 3 mL of toluene and PhI was added (105 μL, 0.9 mmol). At the same time, **8$_{Cs}$** (5.7 mg, 0.015 mmol) was weighted in a crimped vial, dissolved in 1 mL of THF and directly transferred to a syringe of 1 mL and 4.7 mm of diameter. The schlenk and the syringe were taken out of the glovebox. The solution in the schlenk was heated at 95 ºC and stirred at 1200 rpm during 5 min before the addition of the solution of **8$_{Cs}$** in THF started. The syringe containing the solution of **8$_{Cs}$** was placed in a syringe pump covered with aluminum foil. The needle was directly connected to a refrigerated piece of glass (0 ºC) (see Figure S58) with a small cavity inside (6 medium glass and 1.1 mm diameter) that directly aligns the end of the needle to the middle of the solution in the schlenk with a distance between them around 20 cm. Once the set-up is prepared, the solution of **8$_{Cs}$** in THF is pumped with a rate of 0.004 mL/min (around 4 h). When the addition is finished, the mixture is heated 30 min more and then, it is cooled during other 30 min. Afterwards, the solution was filtered through a PTFE 13mm 0.2μm NSTR syringe filter and an aliquot of 1 mL was added to a NMR tube together with the internal standard; fluorobenzene (100 μL of a 0.06 M stock solution in cyclohexane). A ^{19}F NMR spectrum was acquired to determine the yield of benzotrifluoride and the different products obtained for the reaction. The yield was determined by comparing the original mass of CsAg(CF_3)$_2$ (limiting reactive) to its number of moles against the internal standard taking into account that both CF_3 groups are transferred.

The reaction afforded a 56% of benzotrifluoride (**11**) and no catalytically inactive (Xantphos)Pd(CF_3)I. ^{31}P{^{1}H} NMR experiment shows a small amount of the oxidative addition product (Xantphos)Pd(Ph)I and a presumably a Xantphos-oxide compound. It is worth mentioning that this is the first time that product **11** is prepared under catalytic conditions using a Pd$^{0/II}$ manifold.

A screening of the rate of the addition, concentration, solvents, additives and other parameters did not give rise any improvement of the yield.

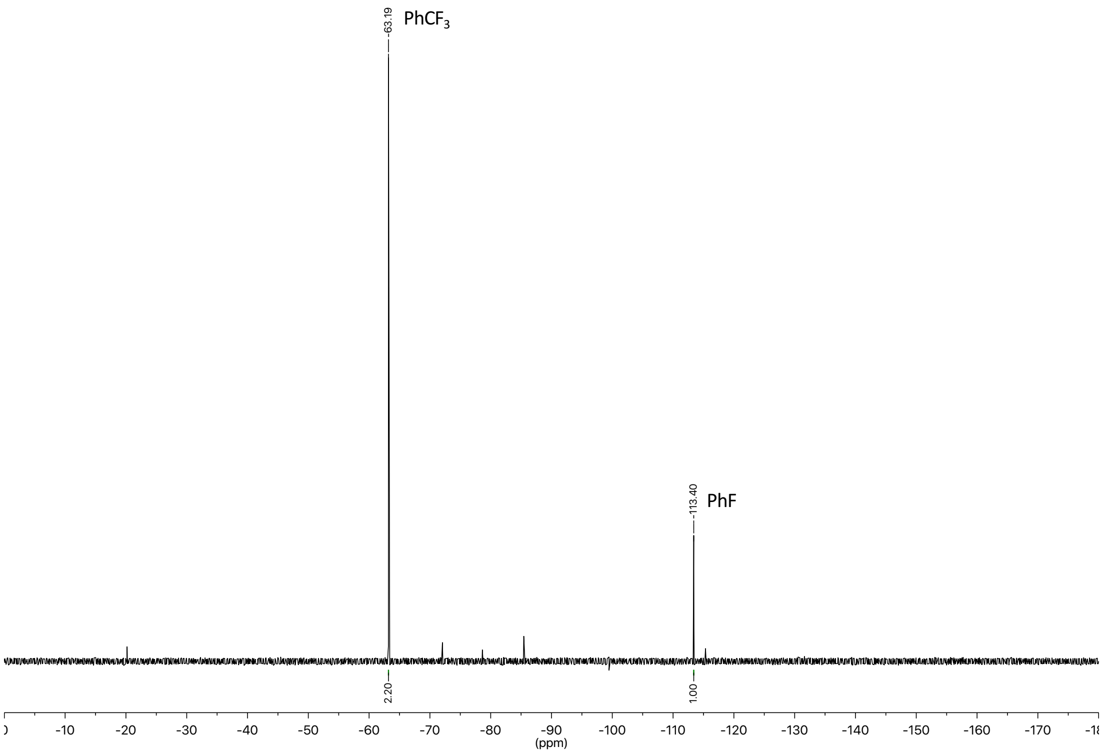


Figure S55. ^{19}F NMR spectrum of the reaction mixture after heating at 95 ºC during 5 h.

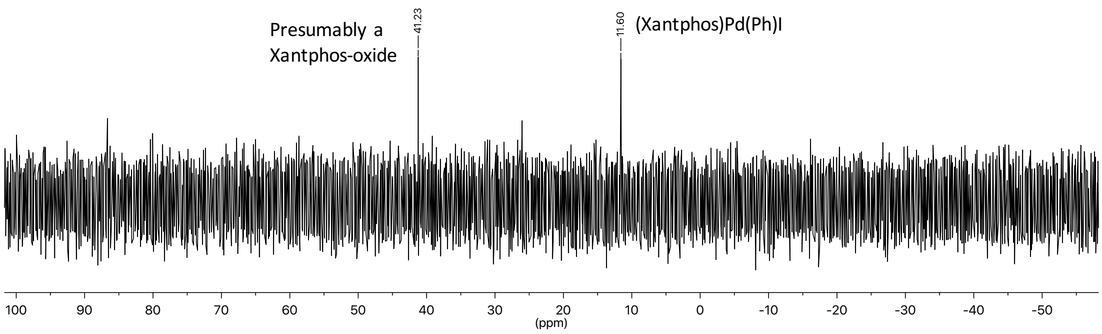


Figure S56. $^{31}P\{1H\}$ NMR spectrum of the reaction mixture after heating at 95 ºC during 5 h.

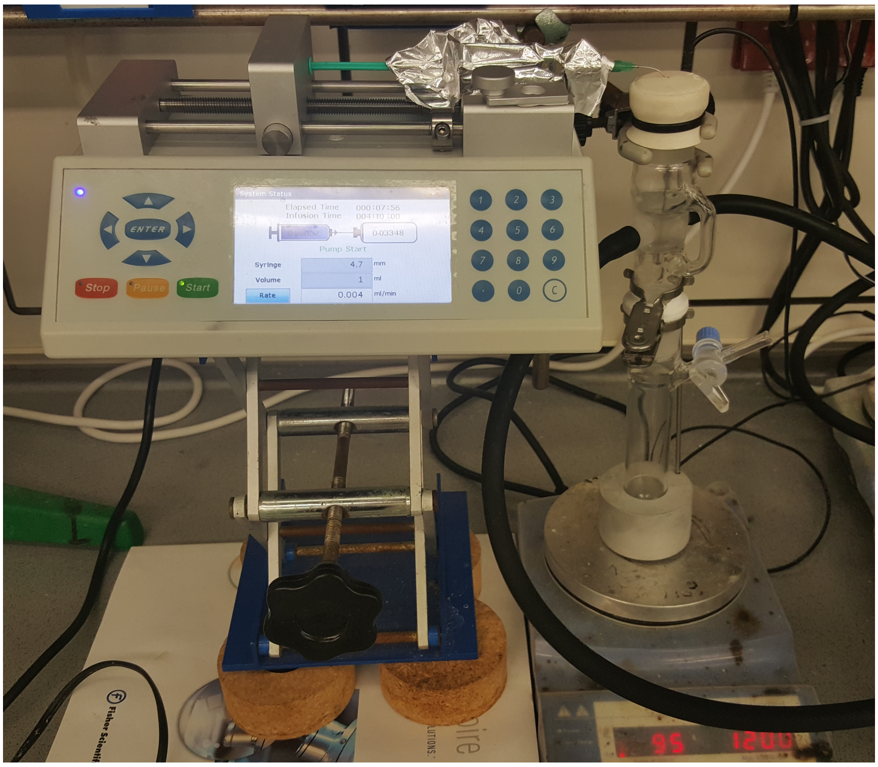


Figure S57. Complete set-up.

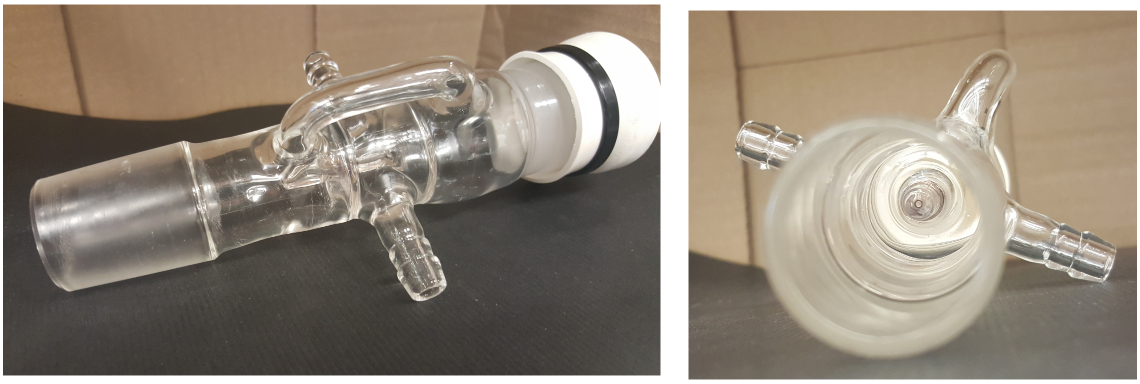


Figure S58. Special piece of glassware

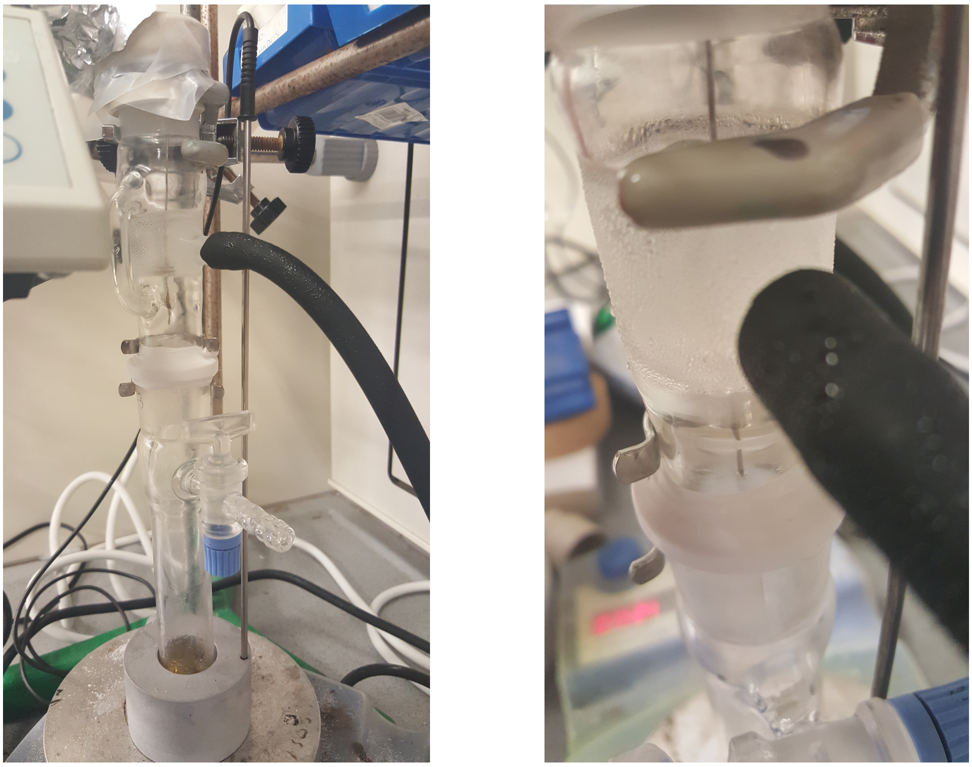


Figure S59. Different pictures of the set-up.

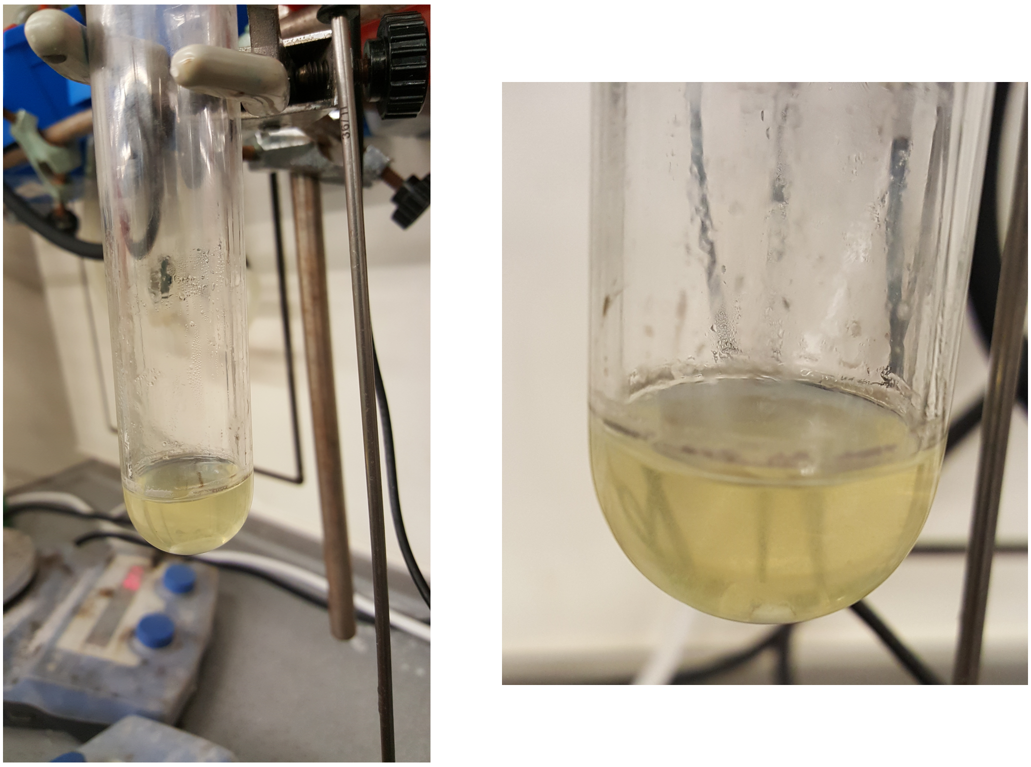


Figure S60. Picture of the reaction after it is finished.

X-ray structure determination for 3, 4a, 5, 6, 7, 8_{Cs}, 8_{NBu_4} and S1.

Crystal preparation: Crystals of **3**, **4a** and **6** were grown by slow diffusion of hexane into solutions of tetrahydrofuran at room temperature. Crystals of **5** and **S1** were grown by slow diffusion of hexane into solutions of dichloromethane at room temperature. Crystals of **7** were grown by slow diffusion of *p*-xylene into a solution of tetrahydrofuran at room temperature. Crystals of $\mathbf{8_{Cs}}$ were grown by slow diffusion of hexane into a solution of tetrahydrofuran at –32 ºC. Crystals of $\mathbf{8_{NBu_4}}$ were grown by slow diffusion of heptane into a solution of tetrahydrofuran at –32 ºC. The measured crystals were prepared under inert conditions, immersed in perfluoropolyether as protecting oil on a glass slide before being mounted on a capton loop. The crystals were handled quickly before being mounted. Compound $\mathbf{8_{Cs}}$ and $\mathbf{8_{NBu_4}}$was crystallized at –32 ºC and the single crystal preparation was performed using dry ice CO_2 as preparation base for avoiding heating of the crystal and mounted at –173 ºC for measurement.

Data collection: Crystal structure determinations for samples **4a**, **6**, **7**, $\mathbf{8_{Cs}}$, $\mathbf{8_{NBu_4}}$ and **S1** were carried out using an Apex DUO Kappa 4-axis goniometer equipped with an APPEX 2 4K CCD area detector, a Microfocus Source E025 IuS using MoK_{α} radiation (0.71073 Å), Quazar MX multilayer Optics as monochromator and an Oxford Cryosystems low temperature device Cryostream 700 plus (T = –173 ˚C). Crystal structure determination for samples **3** and **5** was carried out using a Rigaku diffractometer equipped with a Pilatus 200K area detector, a Rigaku MicroMax-007HF microfocus rotating anode with MoK_{α} radiation, Confocal Max Flux optics and an Oxford Cryosystems low temperature device Cryostream 700 plus (T = –183 ºC). Full-sphere data collection was used with ω and φ scans. *Programs used:* Bruker Device: Data collection APEX-2[18], data reduction Bruker Saint[19]V/.60A and absorption correction SADABS[20] or TWINABS[21]. Rigaku device: Data collection and reduction with CrysAlisPro[22] and absorption correction with Scale3 Abspack scaling algorithm[23].

Structure Solution and Refinement: Crystal structure solution was achieved using the computer program SHELXT.[24] Visualization was performed with the program SHELXle.[25] Missing atoms were subsequently located from difference Fourier synthesis and added to the atom list. Least-squares refinement on F^2 using all measured intensities was carried out using the program SHELXL 2015.[26] All non-hydrogen atoms were refined including anisotropic displacement parameters.

Comments to the structures:

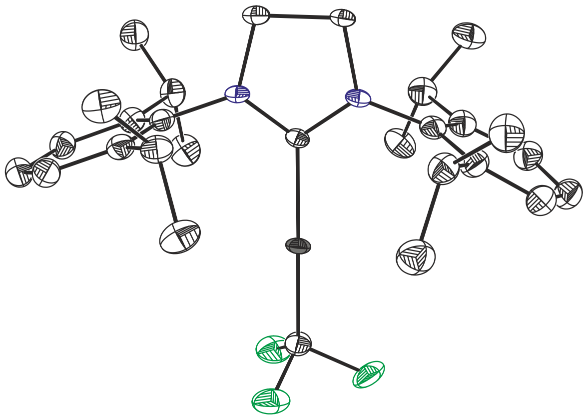


Figure S61. ORTEP drawing (thermal ellipsoids set at 50% probability) of the structure of **3**. Hydrogen atoms have been omitted for clarity.

The asymmetric unit of this compound contains two independent molecules of the metal complex. Both refined molecules are respectively disordered in two shifted positions with ratios of 84:16 and 69:31. The possibility to have a twin (β-angle of 90.84° which may emulate orthorhombic) was checked but the refinement was not successful. The structure is of moderate quality due to the difficulties to find a measurable crystal (A- and B-alerts due to high residual electron densities are commented in the CIF-file).

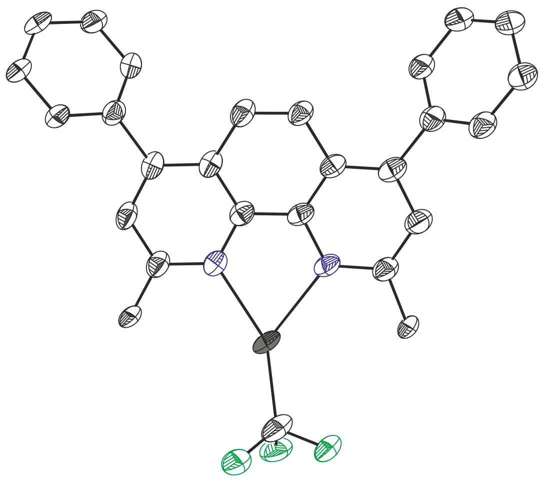


Figure S62. ORTEP drawing (thermal ellipsoids set at 50% probability) of the structure of **4a**. Hydrogen atoms have been omitted for clarity.

The data collected for this structure are of very low quality since the crystals are showing weak diffraction power and the typical signals of high mosaicity. A and B alerts are obtained in the check-cif related to low resolution, poor data to parameter ratio and low bond precision. The following comments were added into the CIF-file in relation to A- and B-alerts: Several crystals of this sample where measured and no better dataset could be collected. The final data collected are showing weak diffraction power and the typical signals of high mosaicity. Although the low data quality, it was considered that the data were good enough for structure confirmation avoiding any deeper discussion about bond lengths and angles. The measured sample was formed by four crystals with a ratio of 29:29:22:20. The collected data for the crystals were processed with TWINABS taking in account overlapping reflections. We considered that the structure is publishable but only for structure identification.

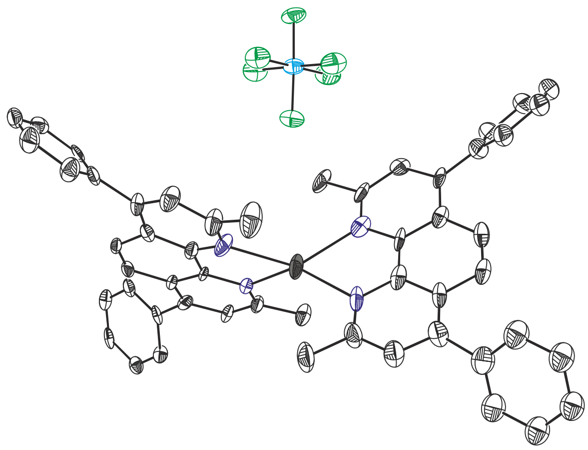


Figure S63. ORTEP drawing (thermal ellipsoids set at 50% probability) of the structure of **5**. Hydrogen atoms have been omitted for clarity.

The asymmetric unit contains two independent cationic molecules of the organometallic compound and two SbF_6 anions. The SbF_6 anions are highly disorder located in three positions. The major part of the aromatic rings at the cationic organometallic compound are disordered in two orientations. The measured crystals were showing a weak diffraction power. Different attempts were performed to collect a complete data set. The final dataset collected was measured on a rotating anode with long exposition time and it was considered of enough quality to confirm the structure.

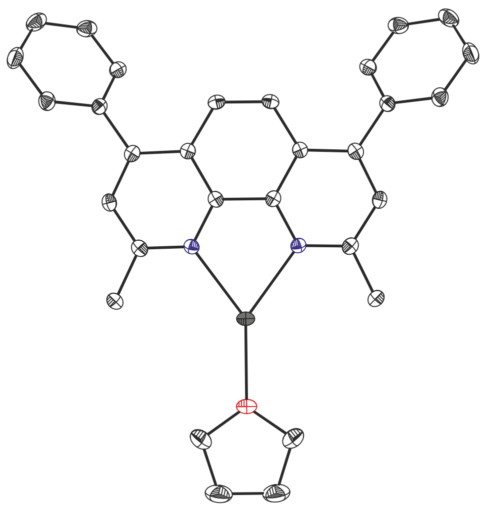


Figure S64. ORTEP drawing (thermal ellipsoids set at 50% probability) of the structure of **6**. Hydrogen atoms and SbF_6 anion have been omitted for clarity.

The asymmetric unit contains a half molecule of the metal complex which shows *C*s-symmetry (mirror plane) and half SbF_6 anion. The THF molecule coordinated to the metal complex is partially disordered in two orientations (ratio of disorder: 65:35).

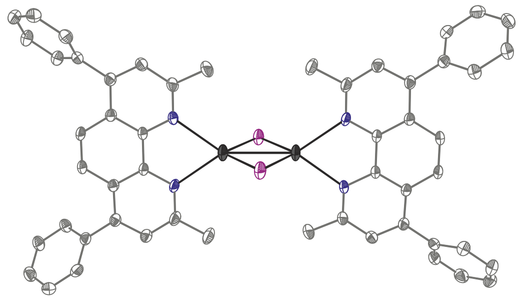


Figure S65. ORTEP drawing (thermal ellipsoids set at 50% probability) of the structure of **7**. Hydrogen atoms and solvent molecules have been omitted for clarity.

The asymmetric unit contains 1/4 molecules of the metal complex (the whole molecule is generated by symmetry operations: mirror plane + 2-fold rotation axes) and 0.375 molecules of *p*-xylene. The solvent amount corresponds 1 ½ molecules of *p*-xylene for each molecule of metal complex. The *p*-xylene molecules are disordered in two positions around a 2-fold rotation axes.

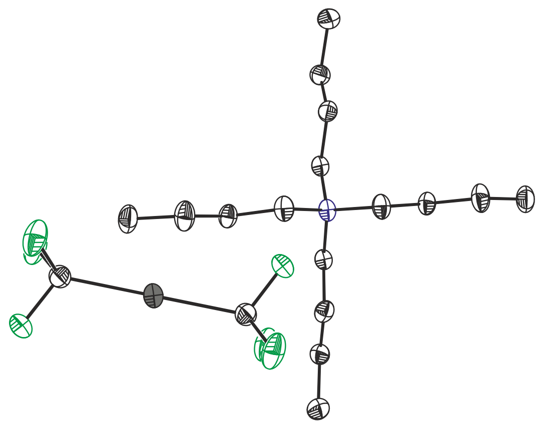


Figure S66. ORTEP drawing showing a fragment of the crystal packing for the structure of $\mathbf{8_{NBu_4}}$ with the thermal ellipsoids set at 50% of probability. Silver atoms are represented grey shaded, carbon atoms with black lines and fluorine atoms with green lines. Hydrogen atoms have been omitted for clarity.

The cation and the anion show *C*2-symmetry in the crystal packing and the asymmetric unit contains only half of each. The fluorine atoms of the CF_3-group are disordered in three orientations with a ratio of 46:44:10.
The silver atom does not show any contact to neighboring silver atoms (7.89 Å). The fluorine atoms do not show any weak interaction and are highly disordered.

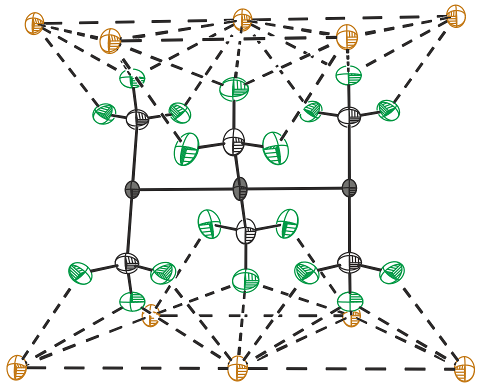


Figure S67. ORTEP drawing showing a fragment of the crystal packing for the structure of **8_{Cs}** with the thermal ellipsoids set at 50% of probability. Silver atoms are represented grey shaded, carbon atoms with black lines, fluorine atoms with green lines and cesium atoms with orange lines.

The asymmetric unit contains half Cs-cation and two quarters of $Ag(CF_3)_2$ anions. All the CF_3 groups are disordered in a minimum of two orientations. The cesium cation is disordered in two positions with a ratio of 57:43. The measured sample is formed by a minimum of two crystals with a ratio of 86:14. The data collected were processed with TWINABS taking in account overlapping reflections. The structure could be refined in the space groups *C*2/m, *C*2 (as a racemic twin) and *C*m (as a twin) with similar results. Finally, the higher symmetrical space group C2/m was selected which also gave the slowest R1 value. Structure solutions were also found using a larger monoclinic unit cell (a:17.00 b:5.77 c:16.12 β:119.57 instead of a:16.12 b:5.77 c:8.35 β:117.60) but the statics were worse so that they were not further used. The selected structure in the space group *C* /2m is of excellent quality and it does not show any A- or B-alerts.

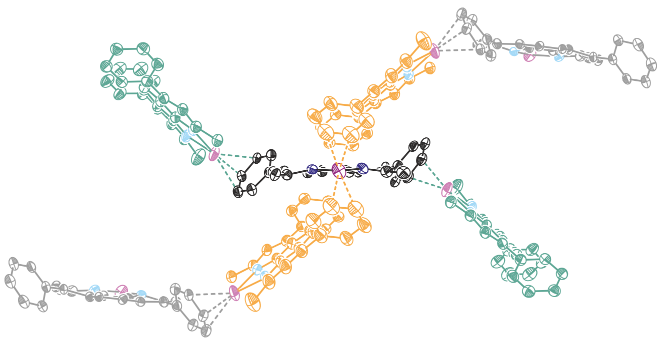
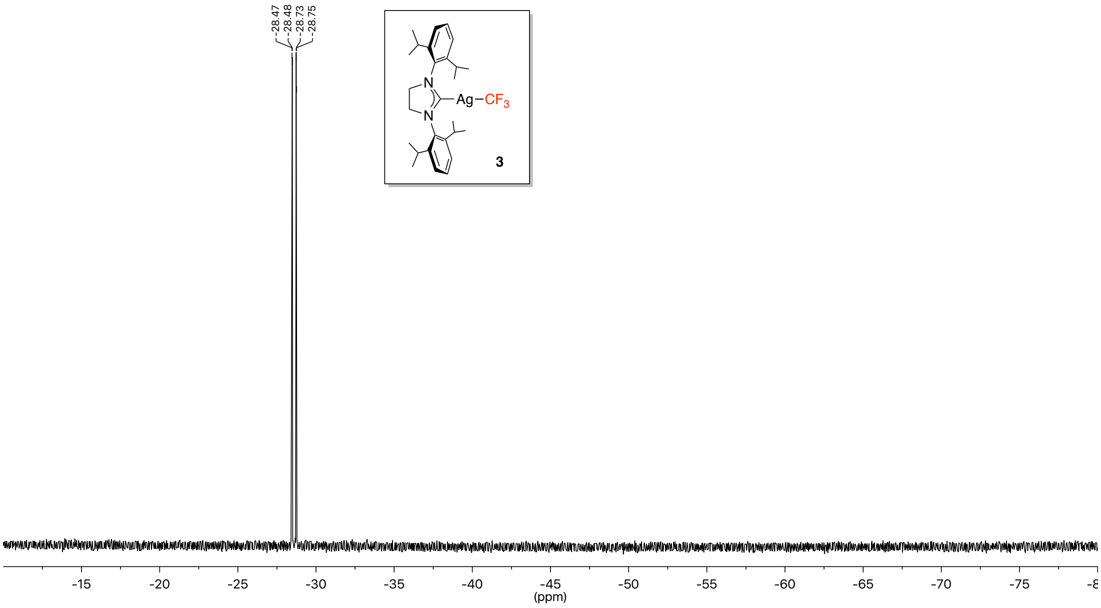


Figure S68. ORTEP drawing showing the interactions in the crystal packing for the structure of **S1** with thermal ellipsoids set at 50% of probability. Hydrogen atoms, solvent molecules and SbF_6 anion have been omitted for clarity.

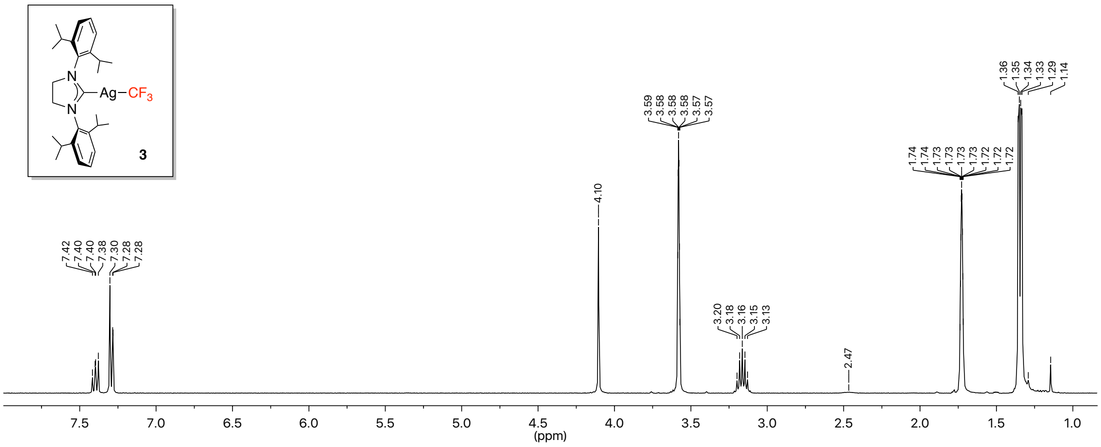
The asymmetric contains one and half molecules of the silver complex cations, one and half SbF_6 anions, a half molecule of dichloromethane and some hexane (see Squeeze). One of the silver metal complex cations and the two SbF_6 anions are disordered in two positions. A highly disordered hexane molecule could not be refined properly. In order to avoid the highly disordered solvent molecule the program SQUEEZE[27] was applied to remove them from the electron density. The obtained crystals were of small dimensions and generally formed by more than one crystal (multicomponent crystals). The finally measured sample was having a weak diffracting power and was formed by two crystals. Since the reflections of both crystals were very close each to one other, the integration was performed using a large box including always the reflections of both crystals. An integration of both crystals dividing the data was not possible. Due to the weak diffraction power, only a reflections-to-parameter ratio of 8:1 was reached. The selected structure refined in the space group $C222_1$ is of good quality (no A-alert and justified B-alerts).

NMR characterization of complex 3

^{19}F NMR spectrum of **3** at 25 ºC (THF-d_8)



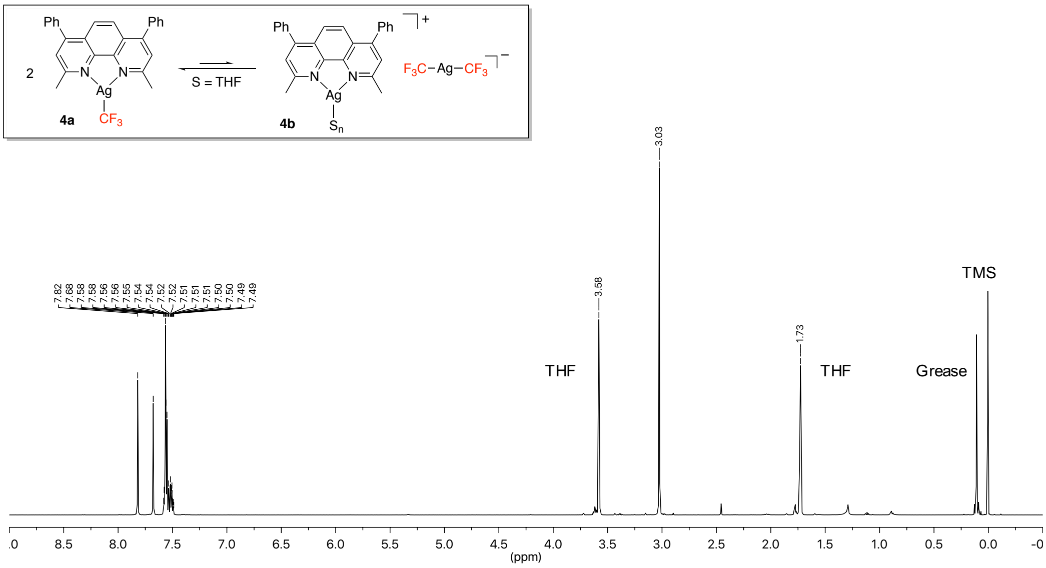
^{1}H NMR spectrum of **3** at 25 ºC (THF-d_8)



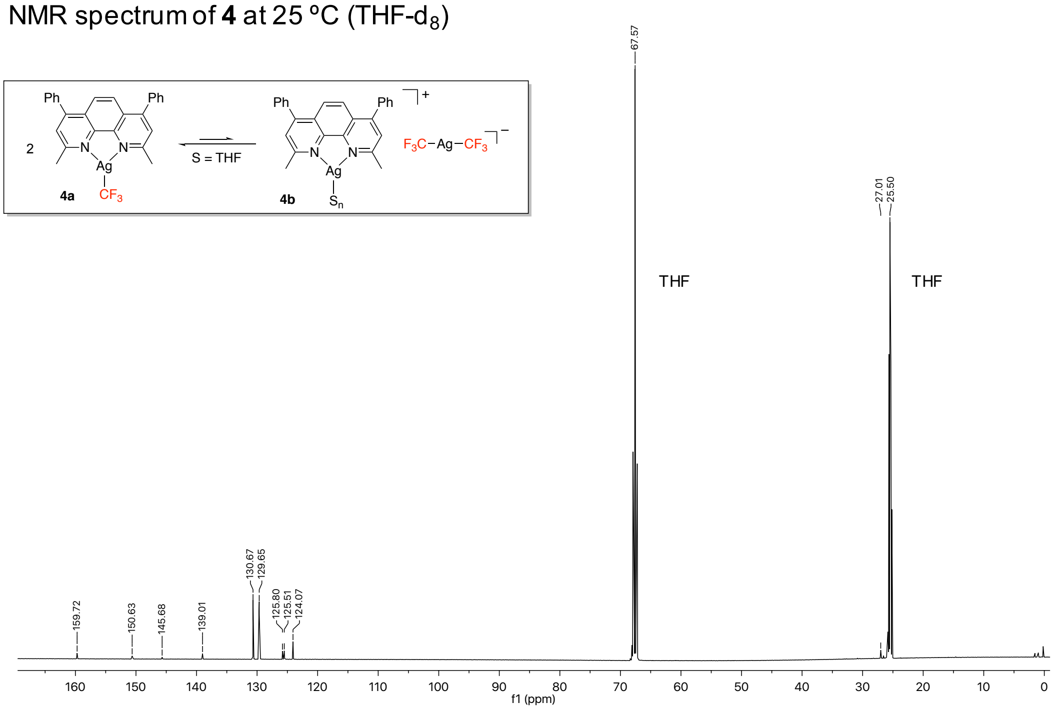
NMR characterization of 4 (4a/4b)

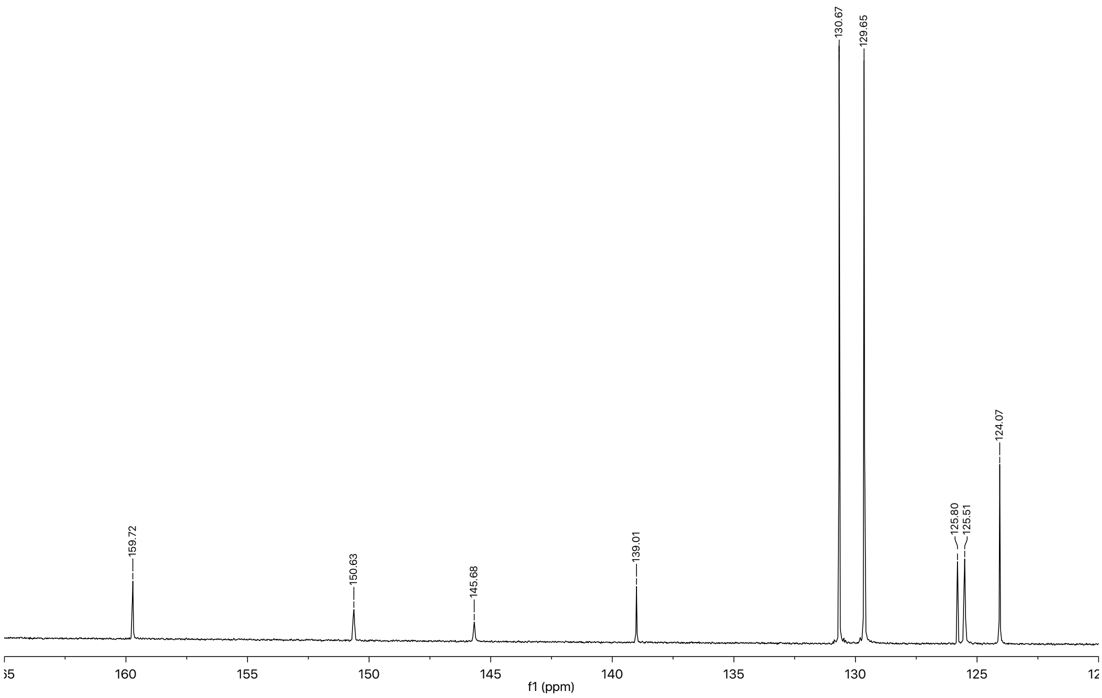
THF

^{1}H NMR spectrum of **4** at 25 °C (THF-d$_8$)

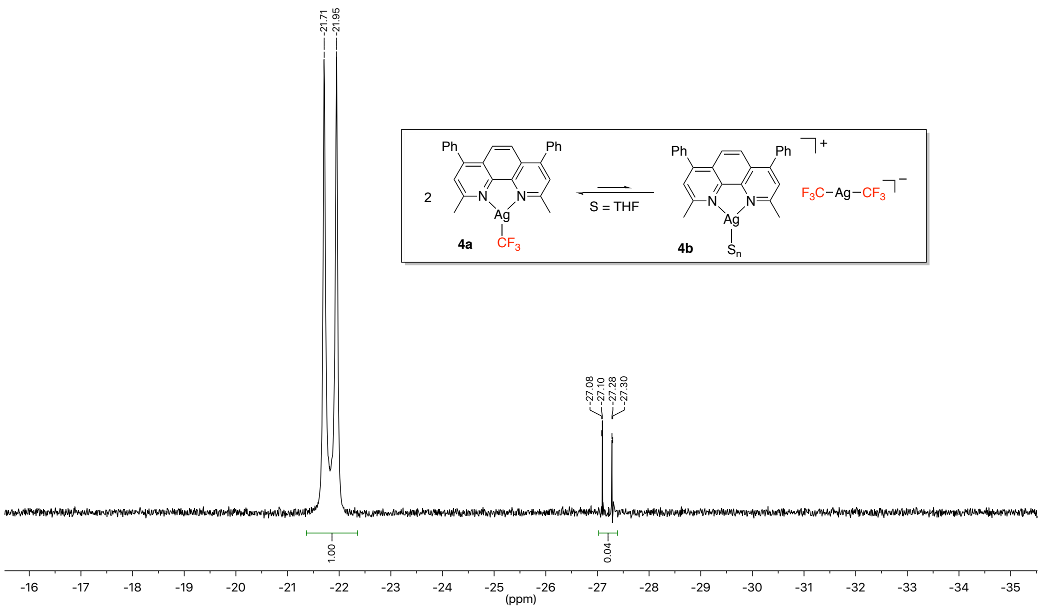


^{13}C NMR spectrum of **4** at 25 °C (THF-d$_8$)

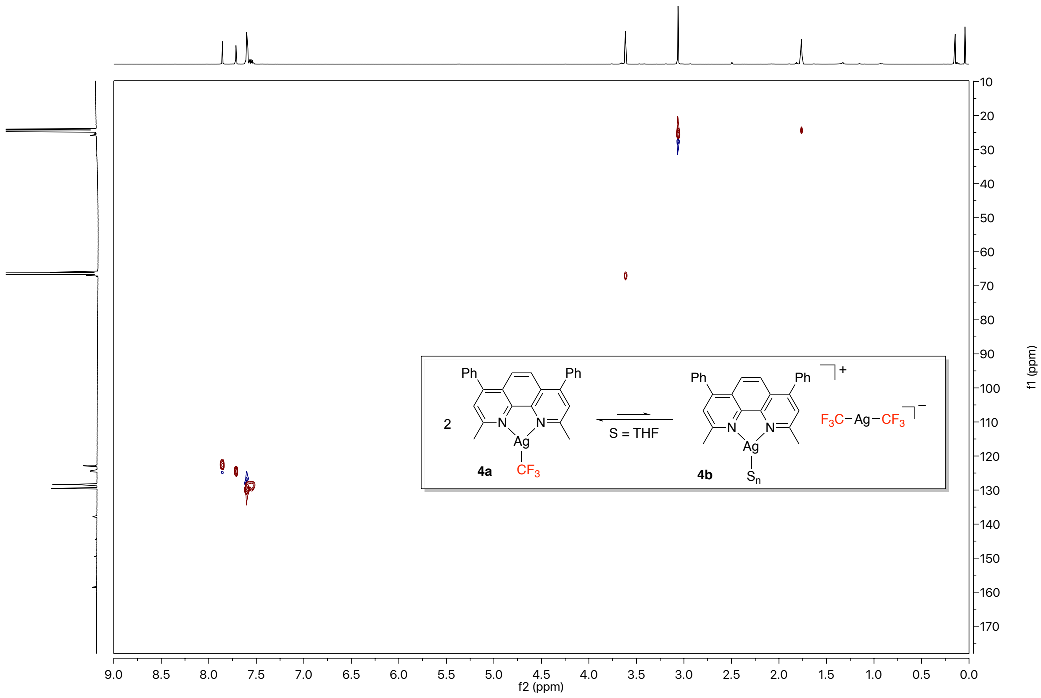




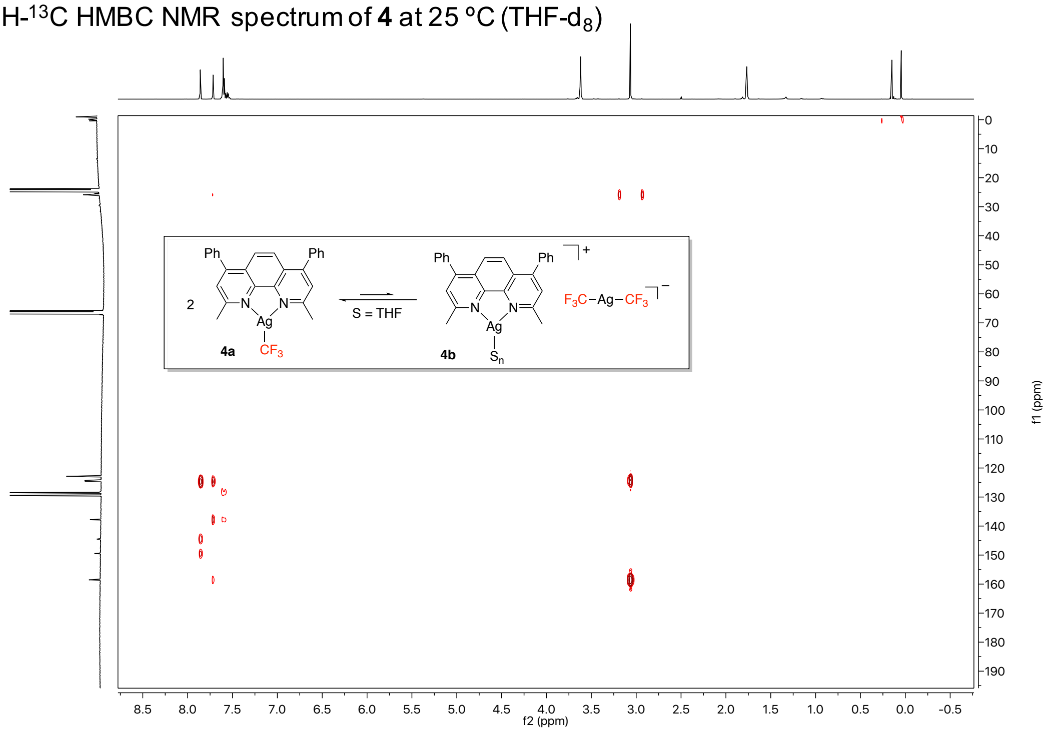
^{19}F NMR spectrum of **4** at 25 °C (THF-d$_8$)



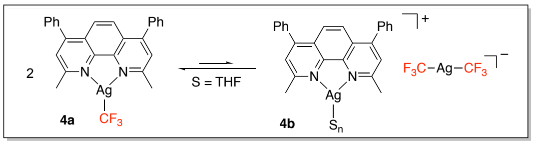
^{1}H-^{13}C HSQC NMR spectrum of **4** at 25 °C (THF-d_8)

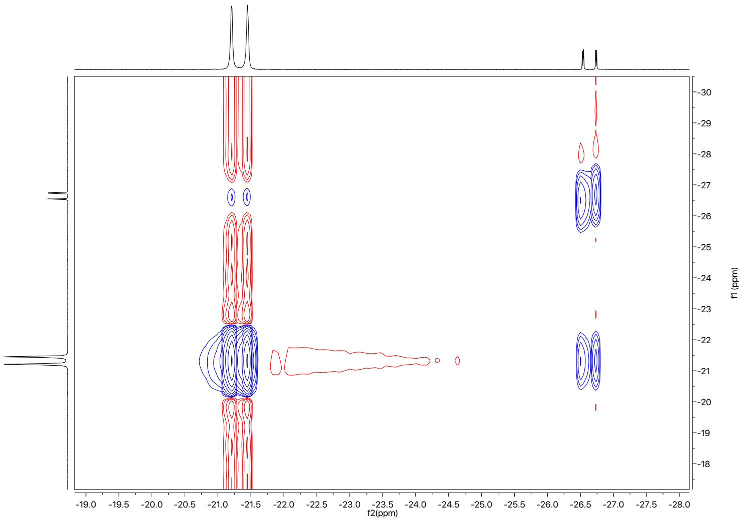


^{1}H-^{13}C HMBC NMR spectrum of **4** at 25 °C (THF-d_8)



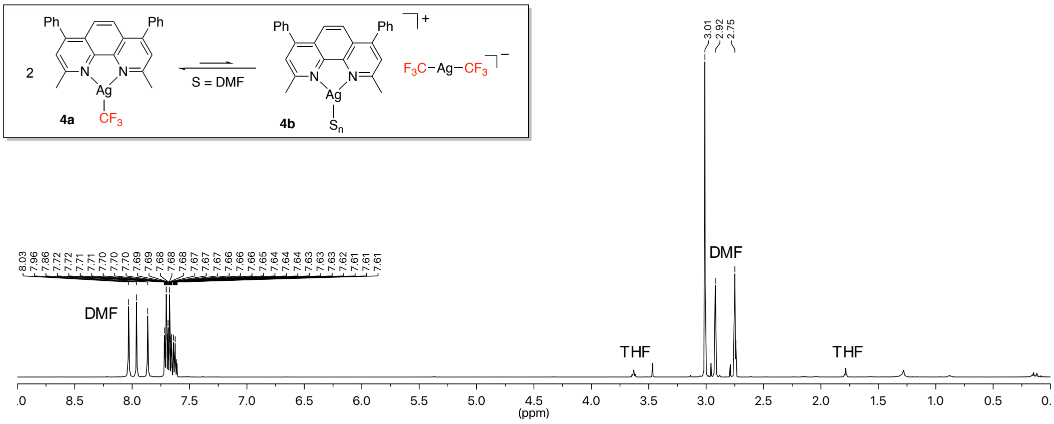
EXSY ^{19}F NMR spectrum of **4** at 25 °C (THF-d_8)



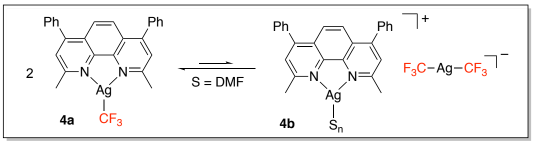


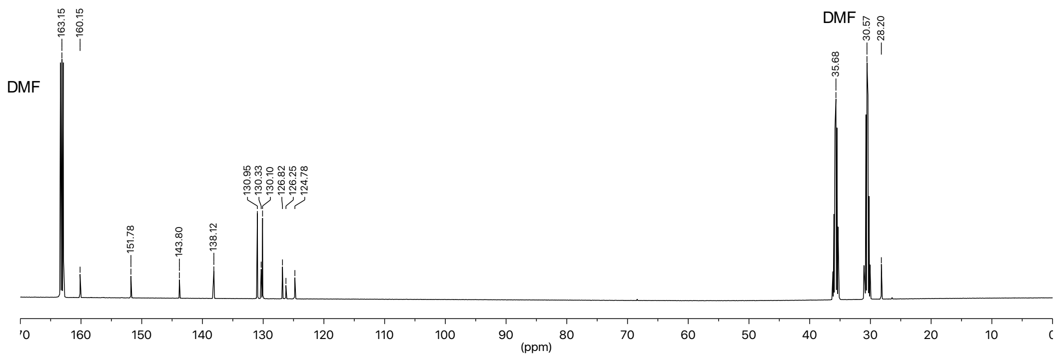
DMF

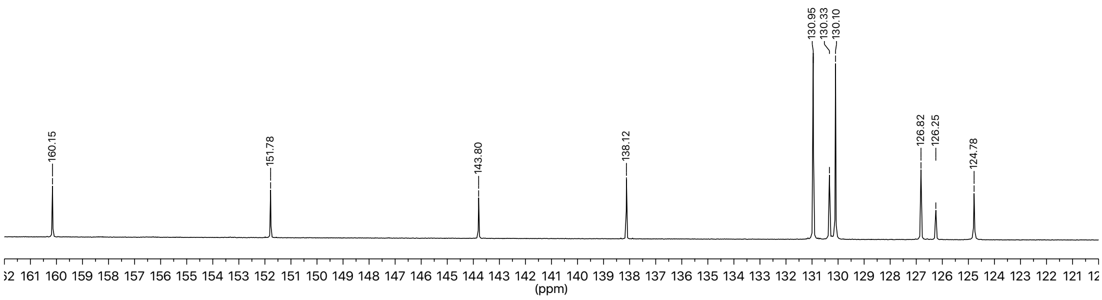
^{1}H NMR spectrum of **4** at 25 °C (DMF-d_7)



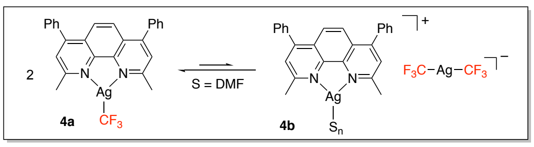
^{13}C NMR spectrum of **4** at 25 °C (DMF-d_7)

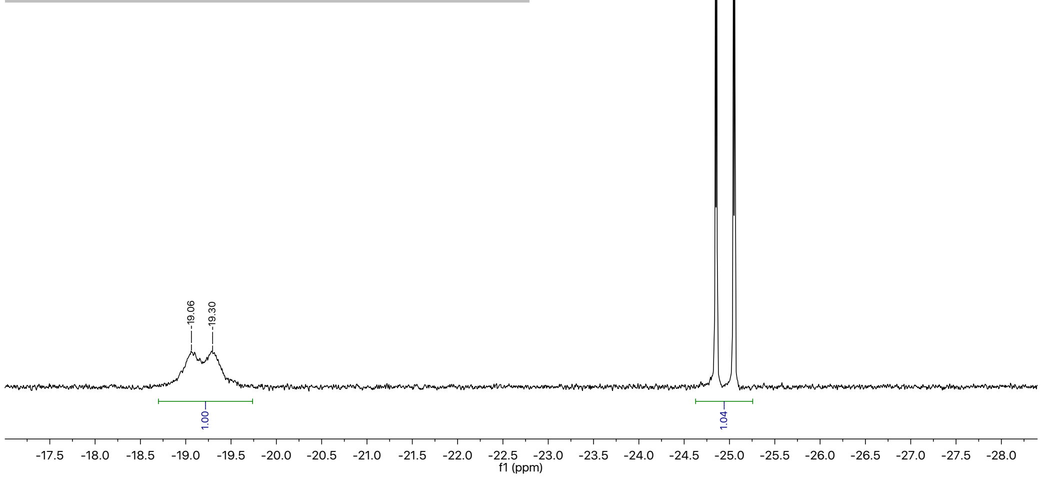




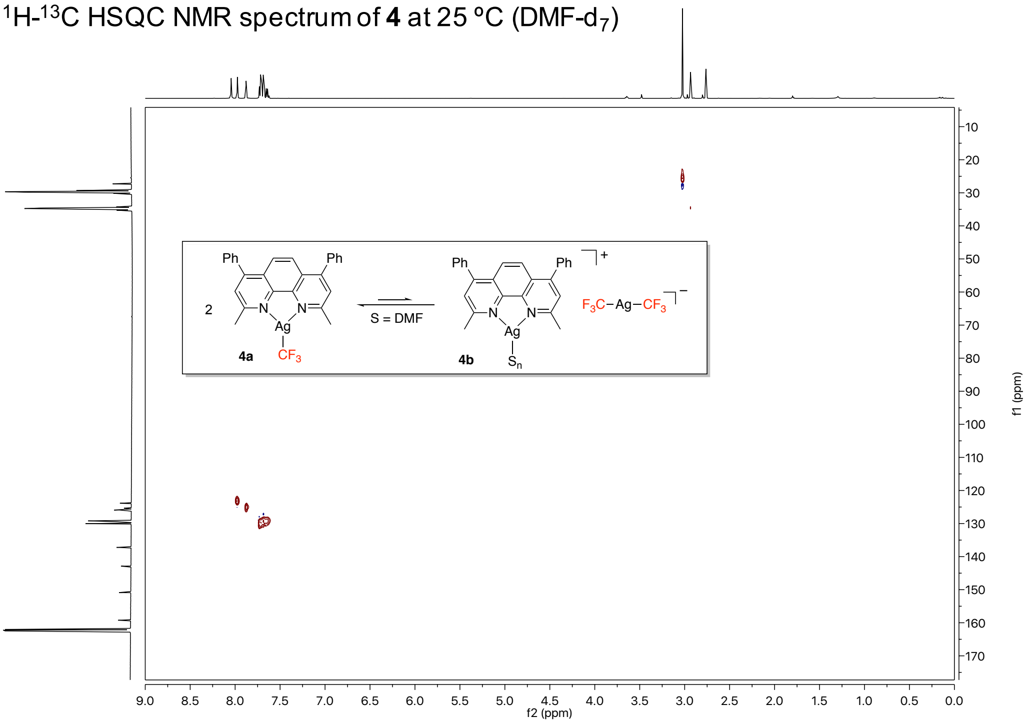


^{19}F NMR spectrum of **4** at 25 °C (DMF-d_7)

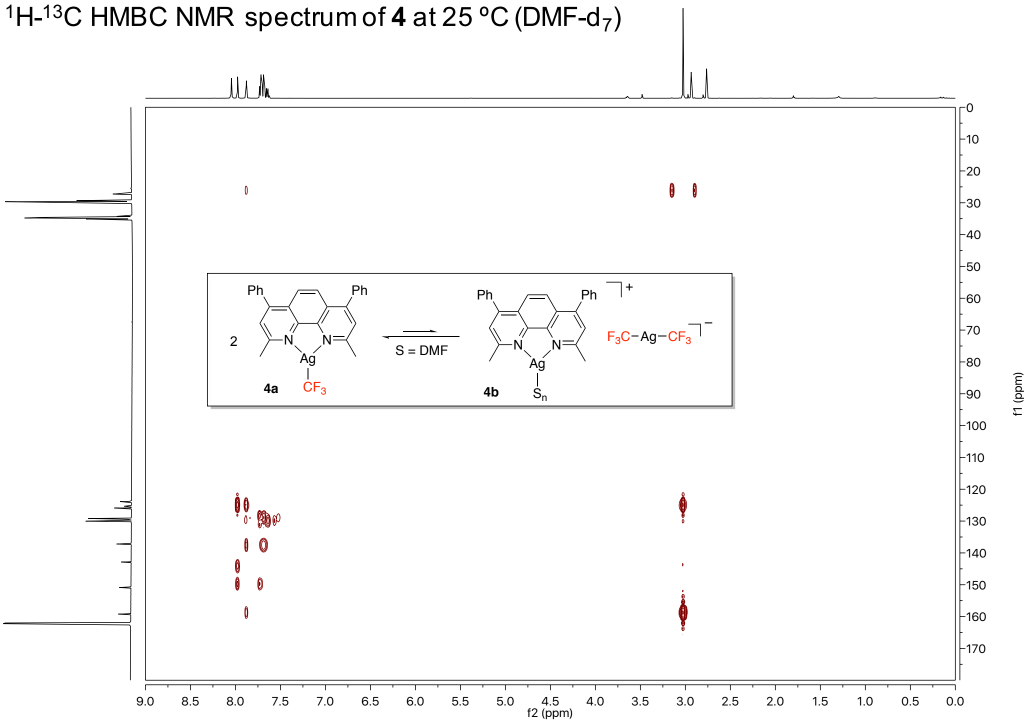




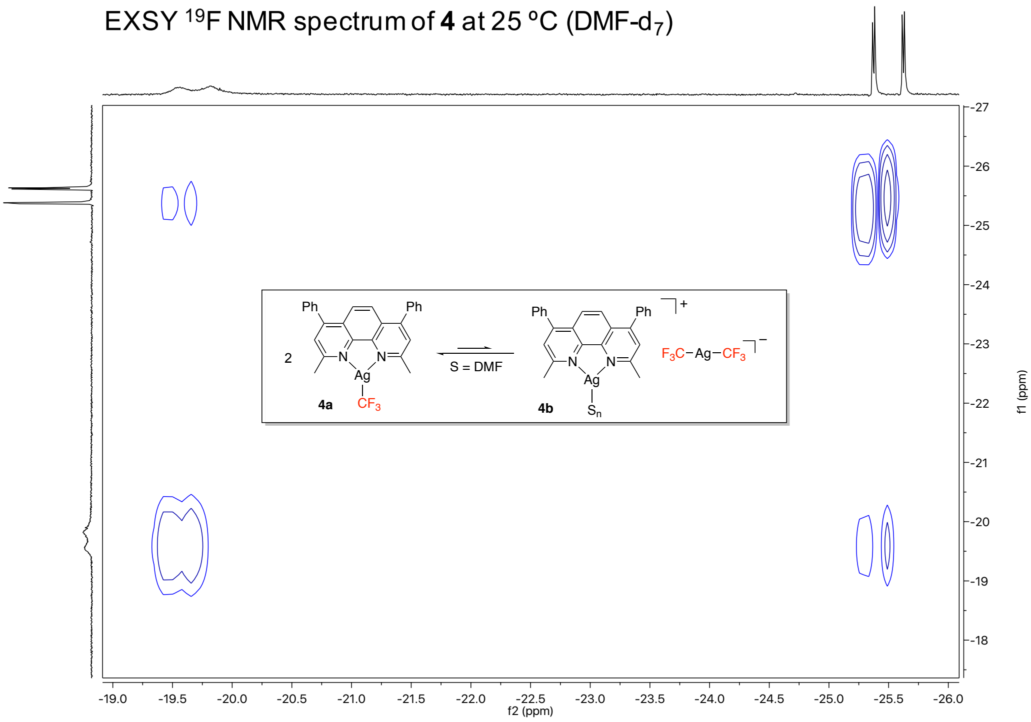
^{1}H-^{13}C HSQC NMR spectrum of **4** at 25 °C (DMF-d_7)



^{1}H-^{13}C HMBC NMR spectrum of **4** at 25 °C (DMF-d_7)

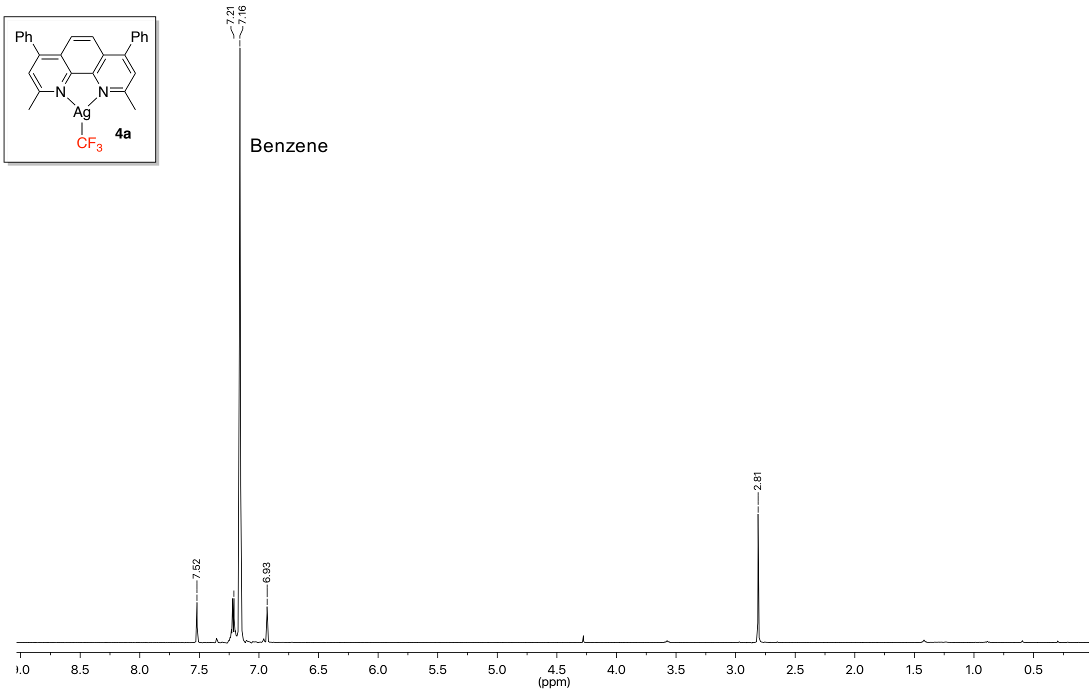


EXSY ^{19}F NMR spectrum of **4** at 25 °C (DMF-d_7)

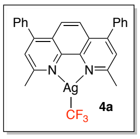


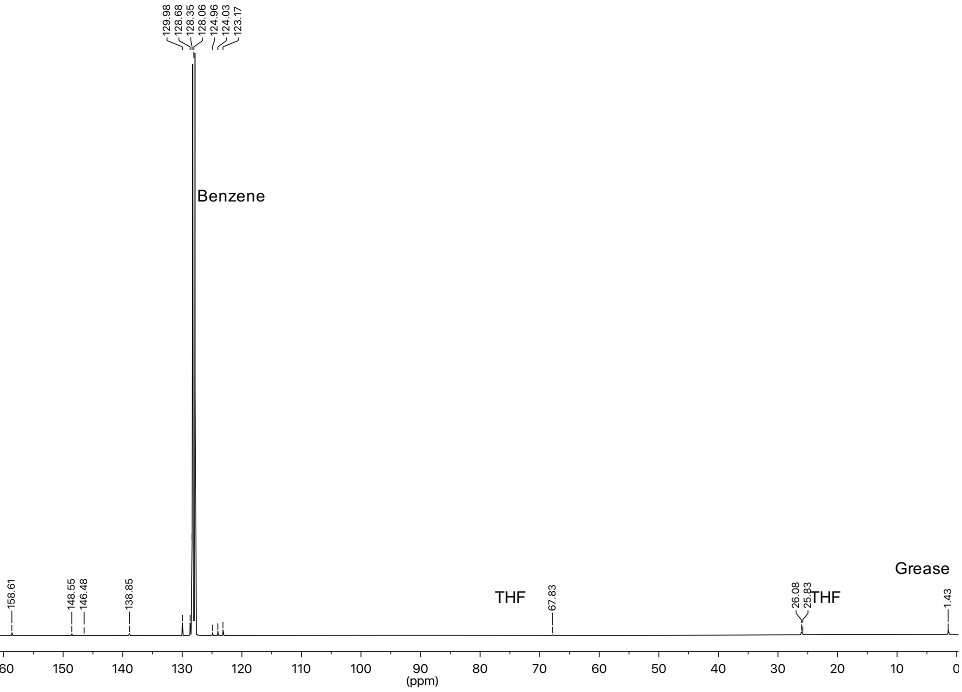
Benzene

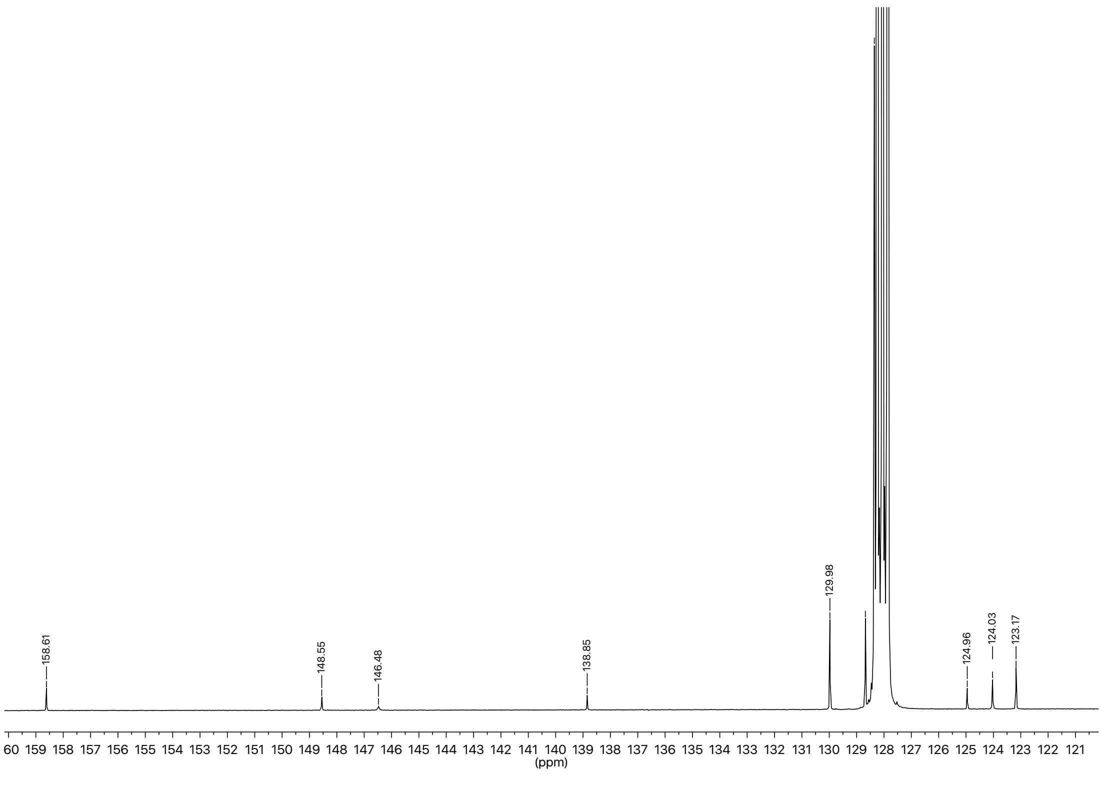
^{1}H NMR spectrum of **4a** at 25 °C (Benzene-d_6)



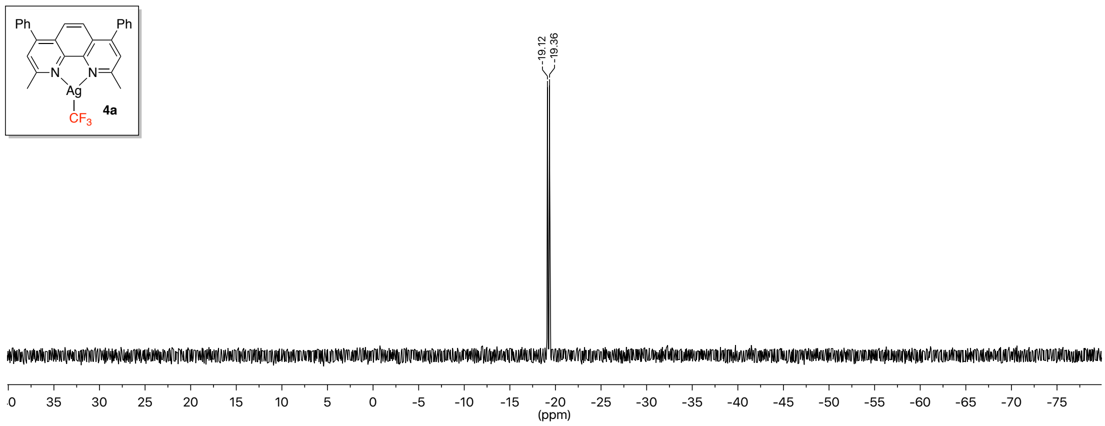
^{13}C NMR spectrum of **4a** at 25ºC (Benzene-d_6)



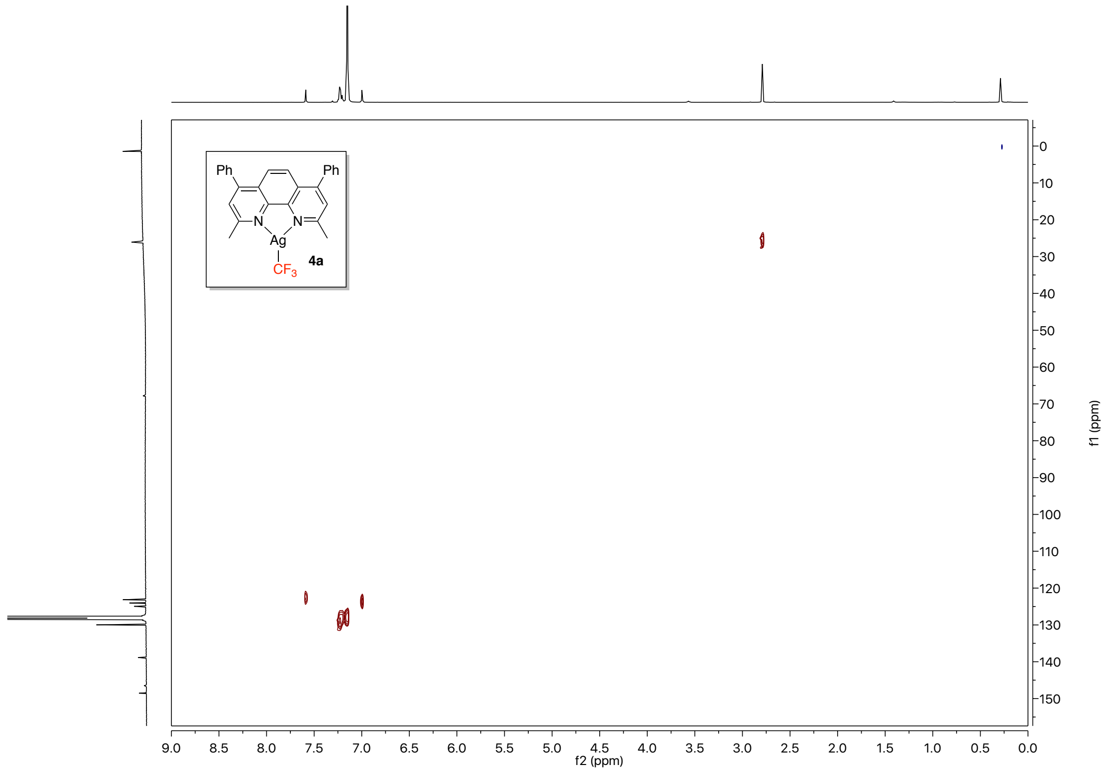




^{19}F NMR spectrum of **4a** at 25 ºC (Benzene-d_6)



^{1}H-^{13}C HSQC NMR spectrum of **4a** at 25 ºC (Benzene-d_6)



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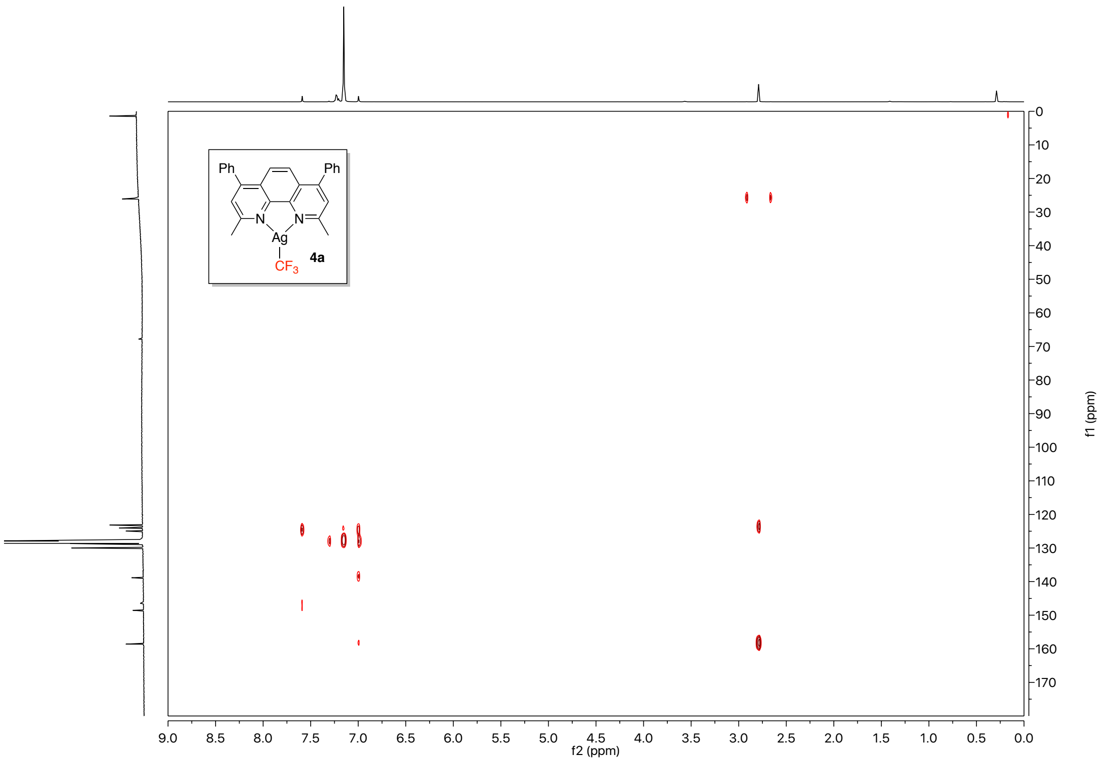
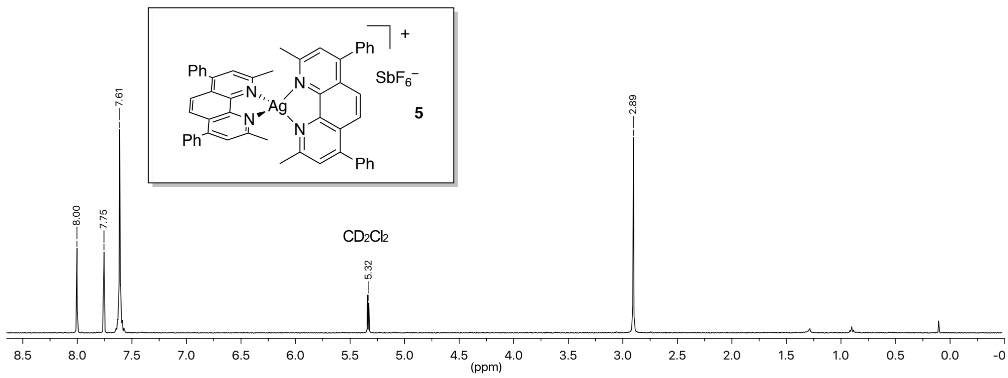


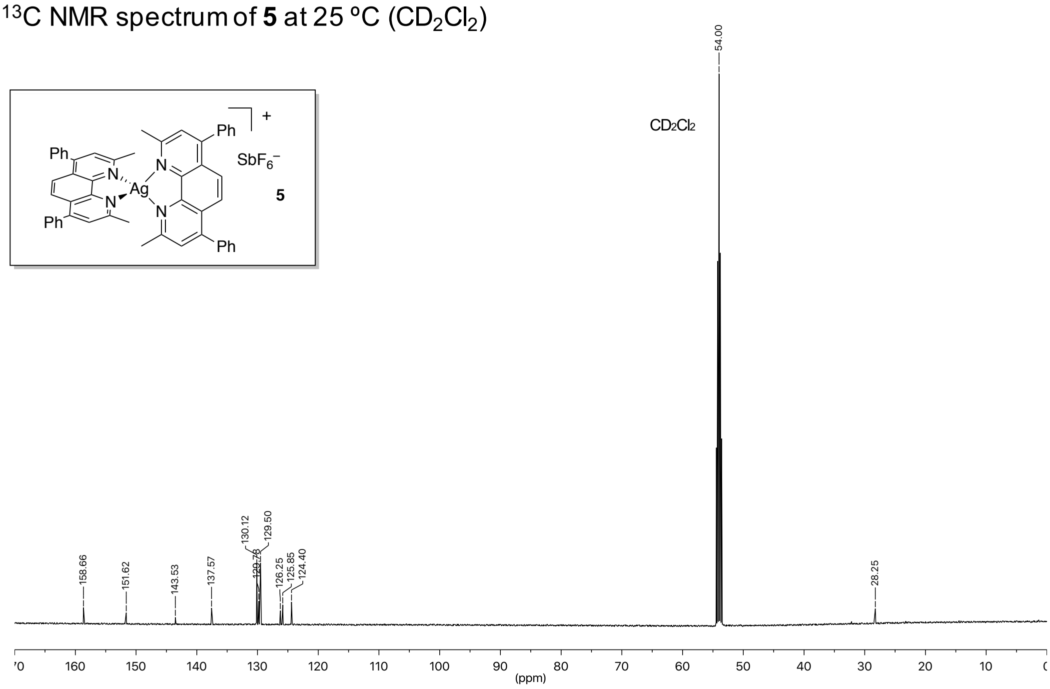
NMR characterization of 5

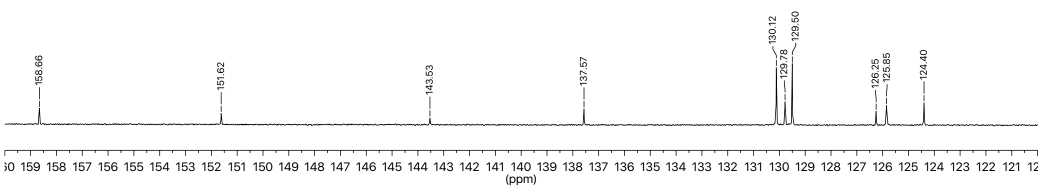
DCM

^{1}H NMR spectrum of **5** at 25 ºC (CD_2Cl_2)

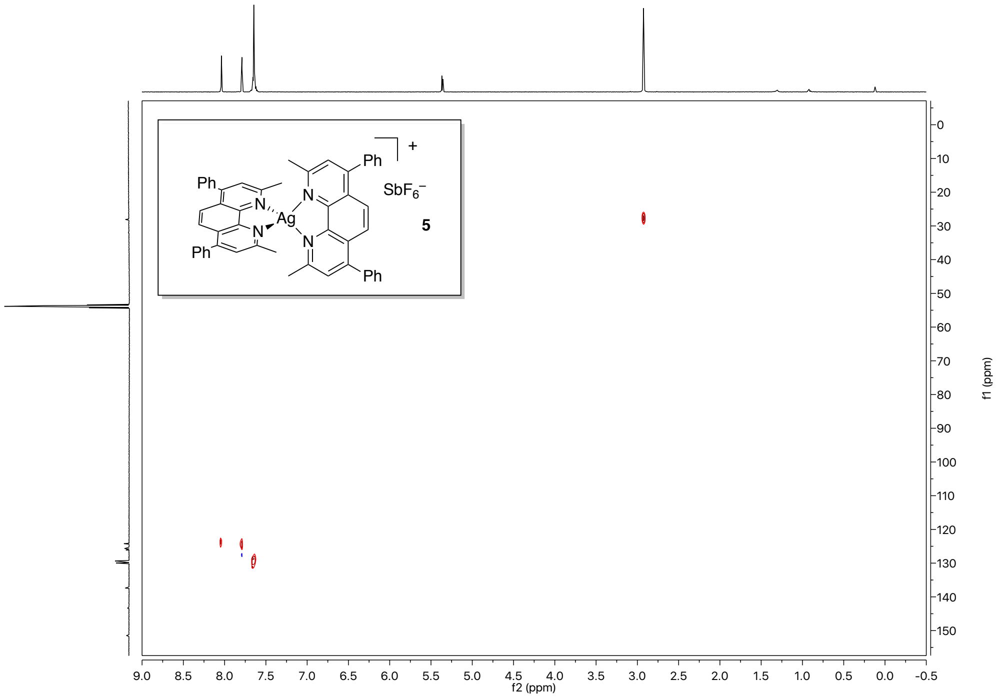


^{13}C NMR spectrum of **5** at 25 ºC (CD_2Cl_2)

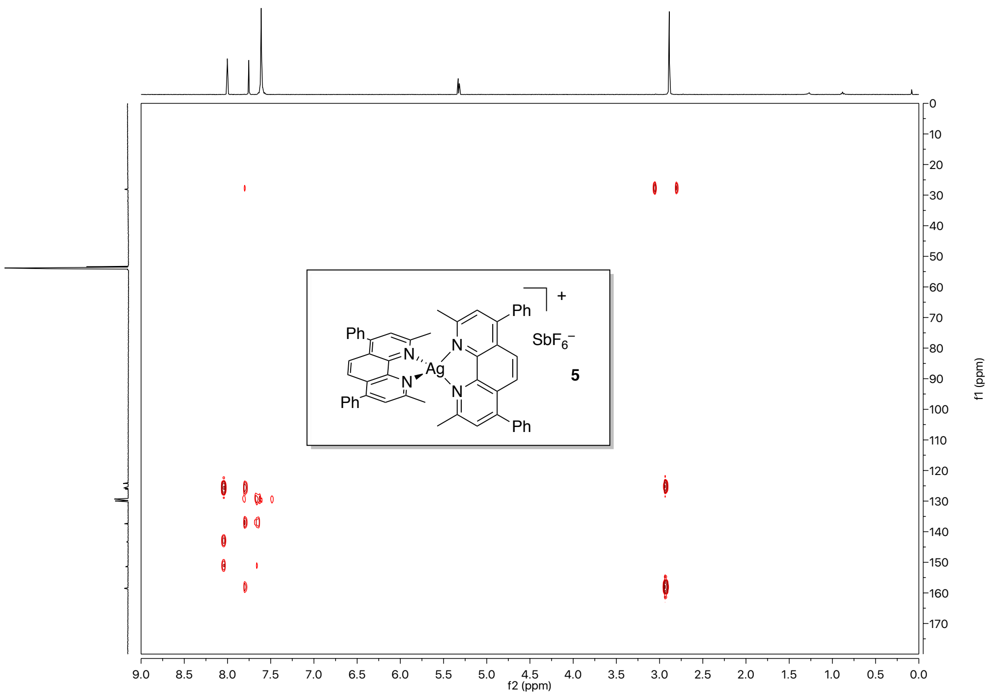




^1H-^{13}C HSQC NMR spectrum of **5** at 25 ºC (CD_2Cl_2)

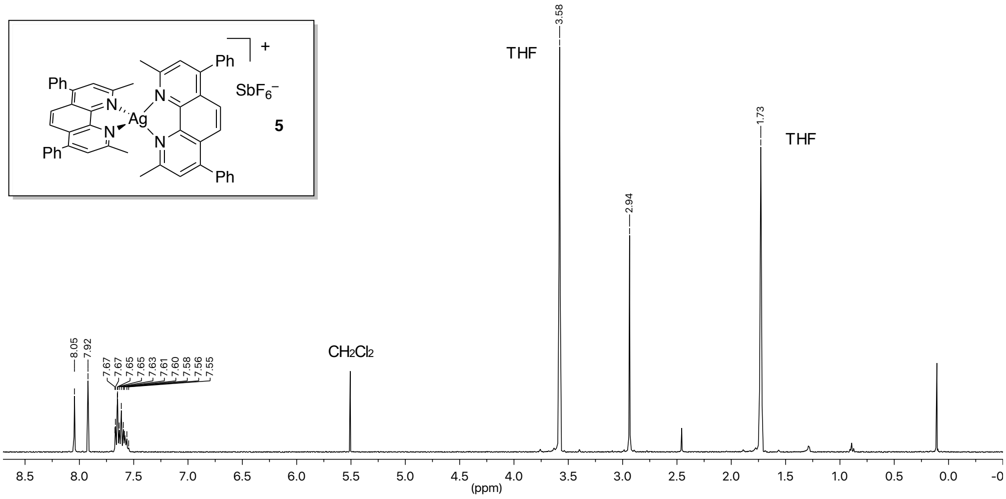


^1H-^{13}C HMBC NMR spectrum of **5** at 25 ºC (CD_2Cl_2)

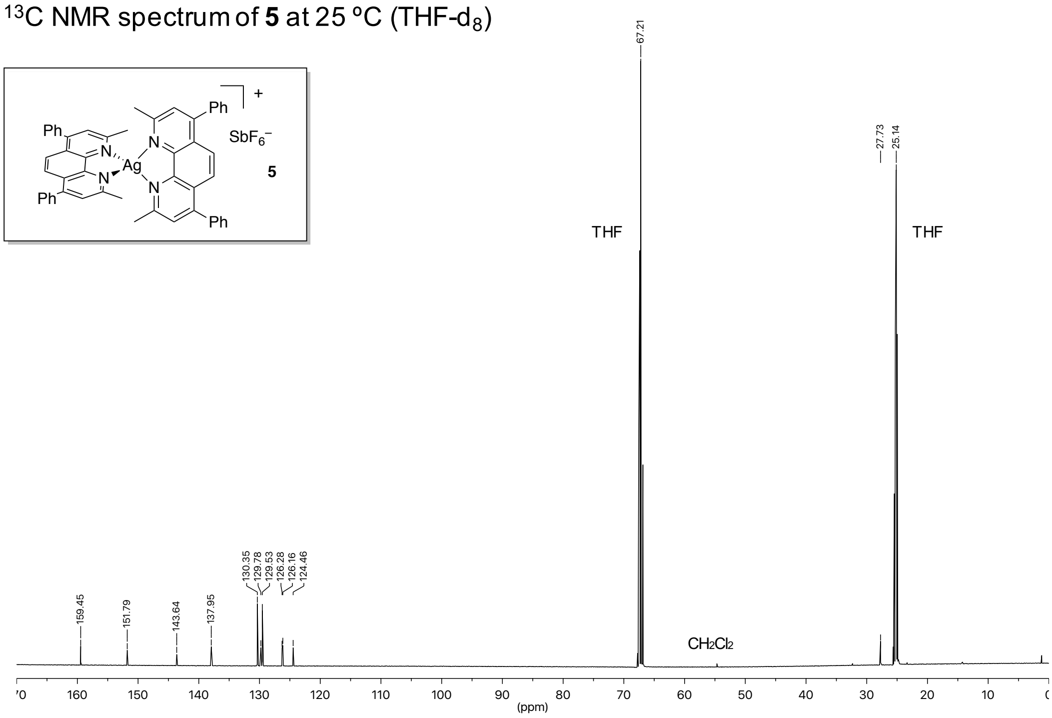


THF

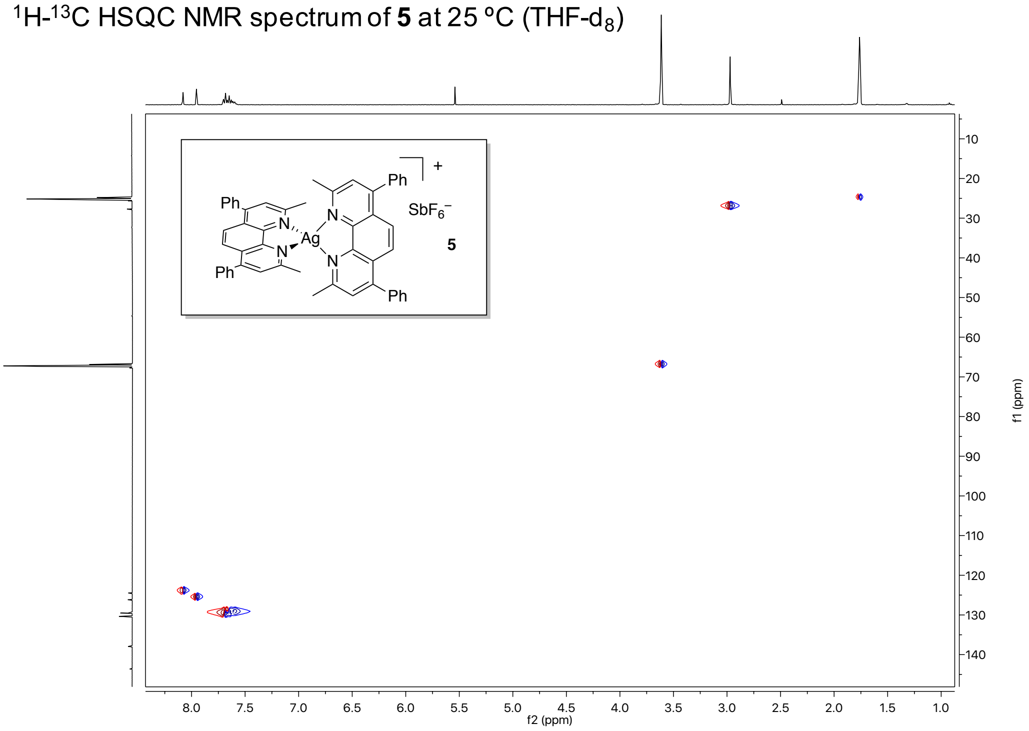
^1H NMR spectrum of **5** at 25 ºC (THF-d_8)



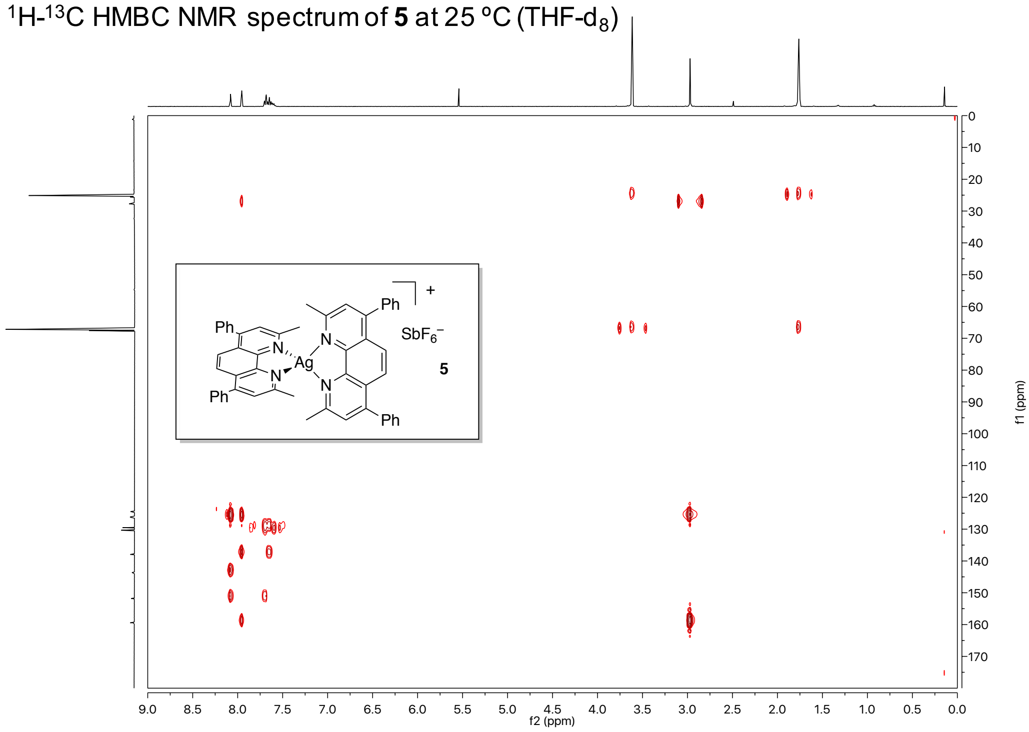
^{13}C NMR spectrum of **5** at 25 ºC (THF-d_8)



^{1}H-^{13}C HSQC NMR spectrum of **5** at 25 °C (THF-d_8)

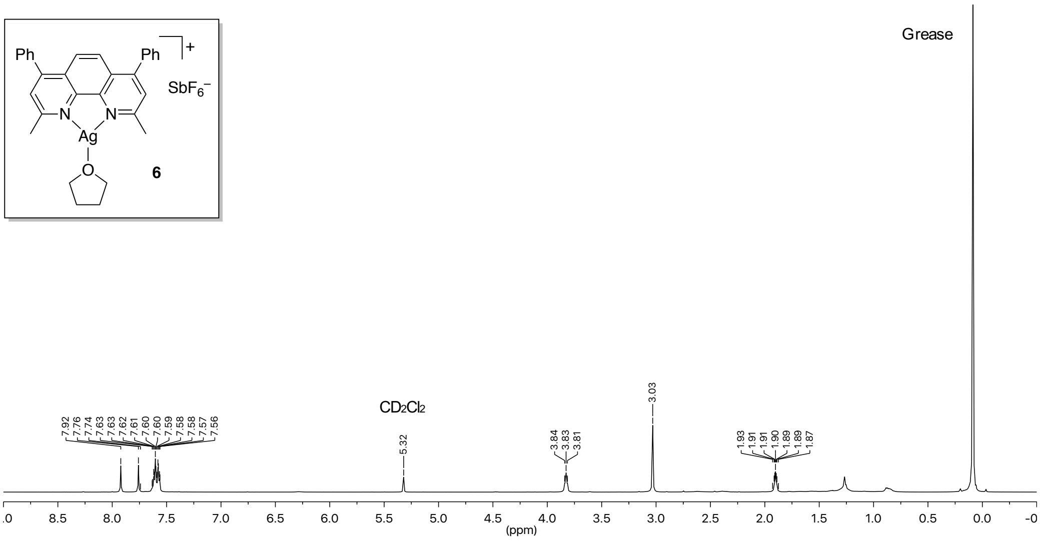


^{1}H-^{13}C HMBC NMR spectrum of **5** at 25 °C (THF-d_8)

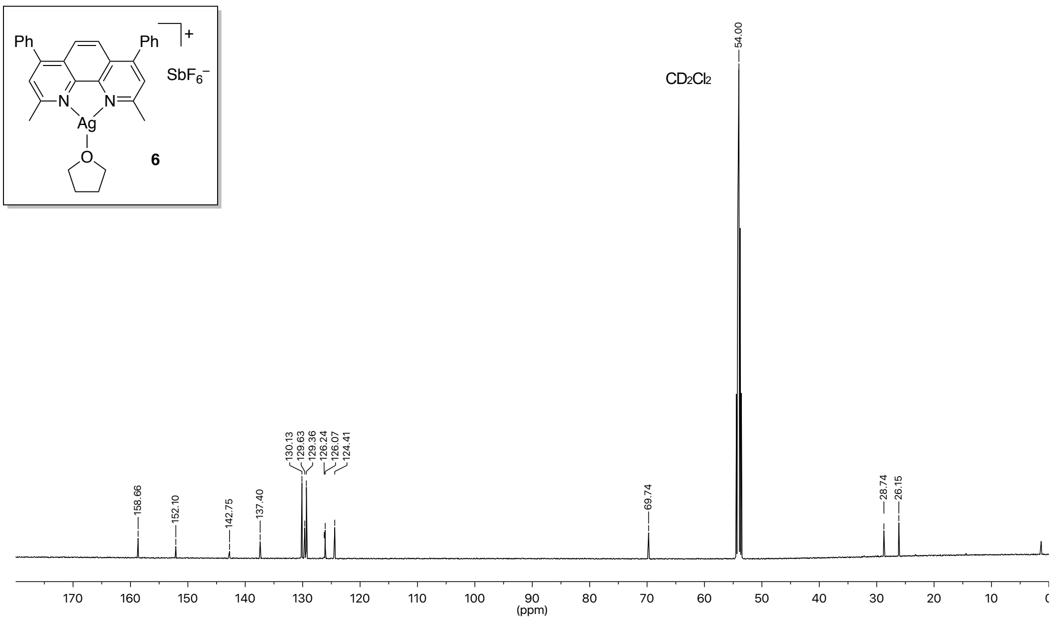


NMR characterization of 6

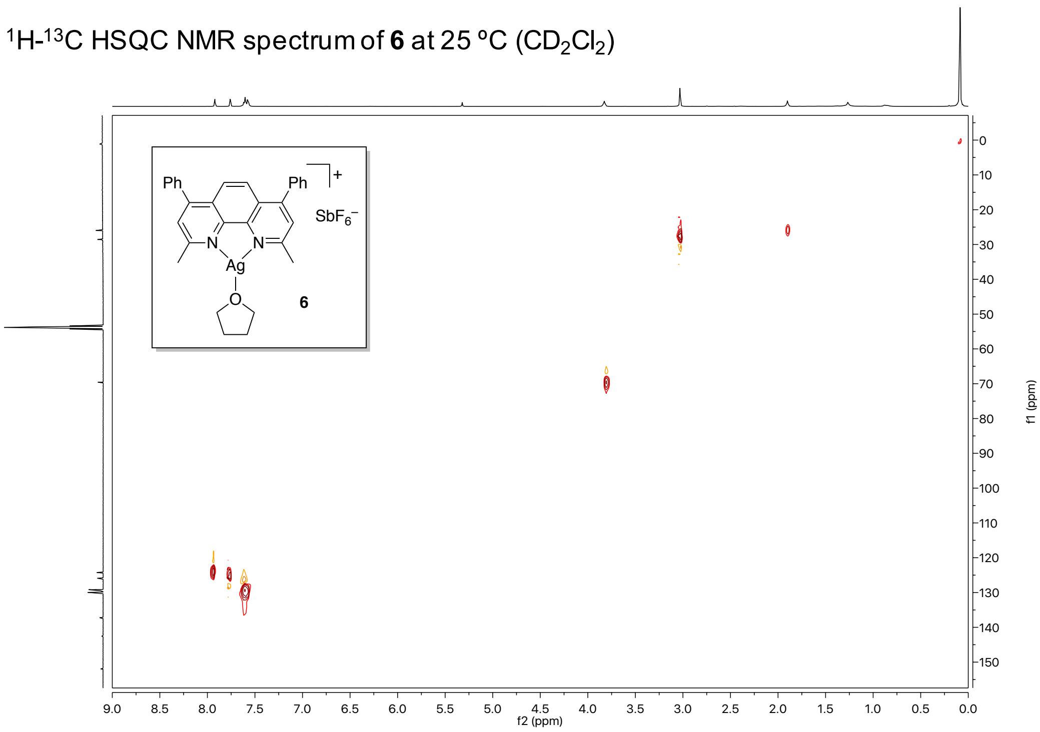
^{1}H NMR spectrum of **6** at 25 ºC (CD_2Cl_2)



^{13}C NMR spectrum of **6** at 25 ºC (CD_2Cl_2)

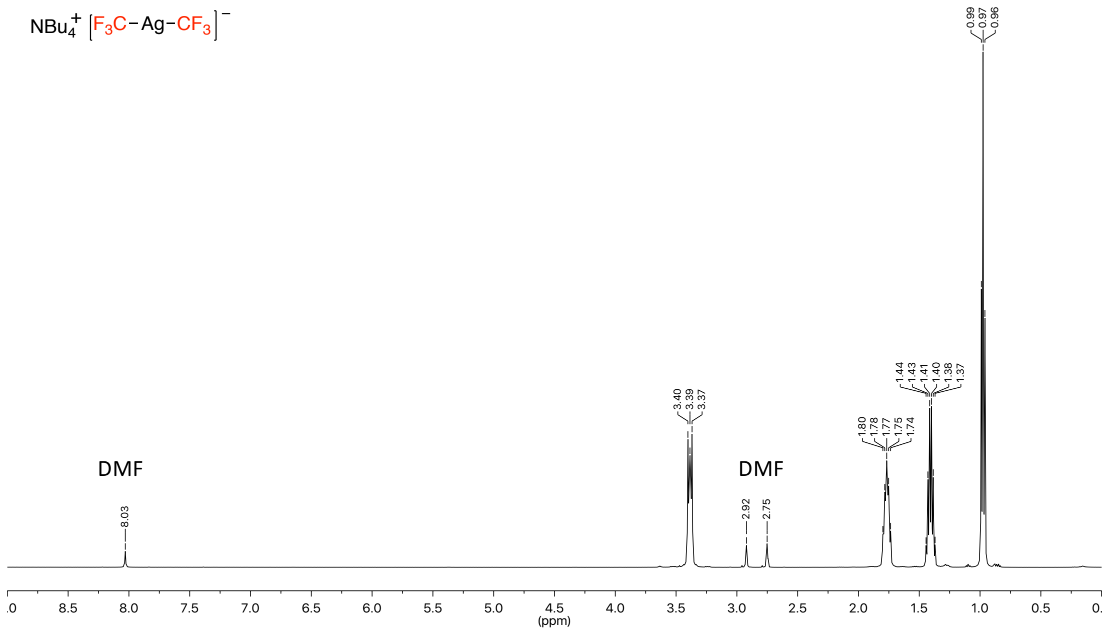


^1H-^{13}C HSQC NMR spectrum of **6** at 25 °C (CD_2Cl_2)

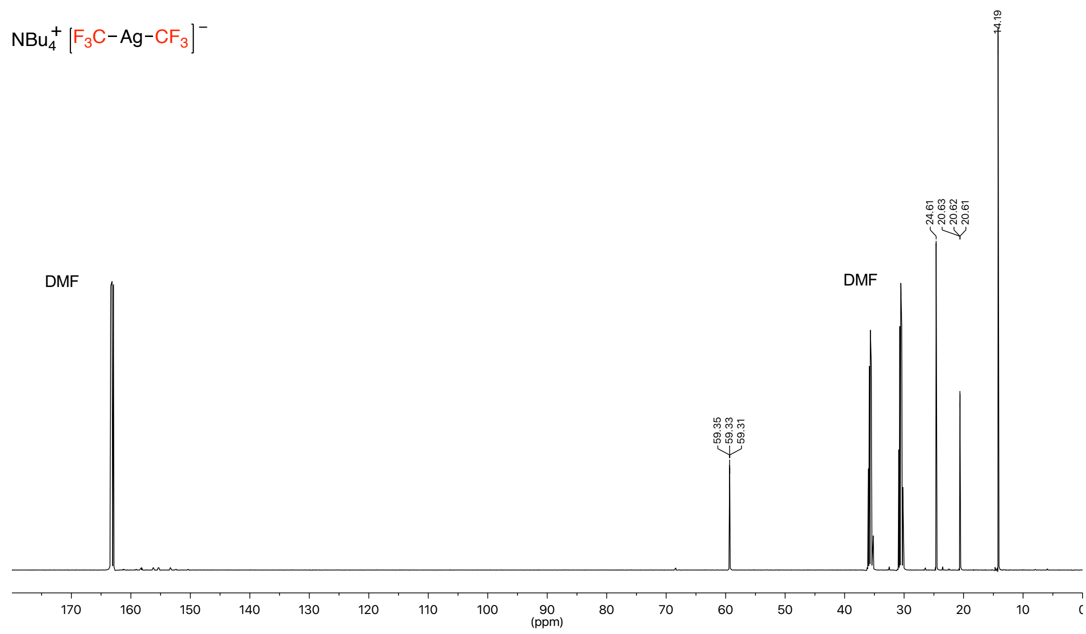


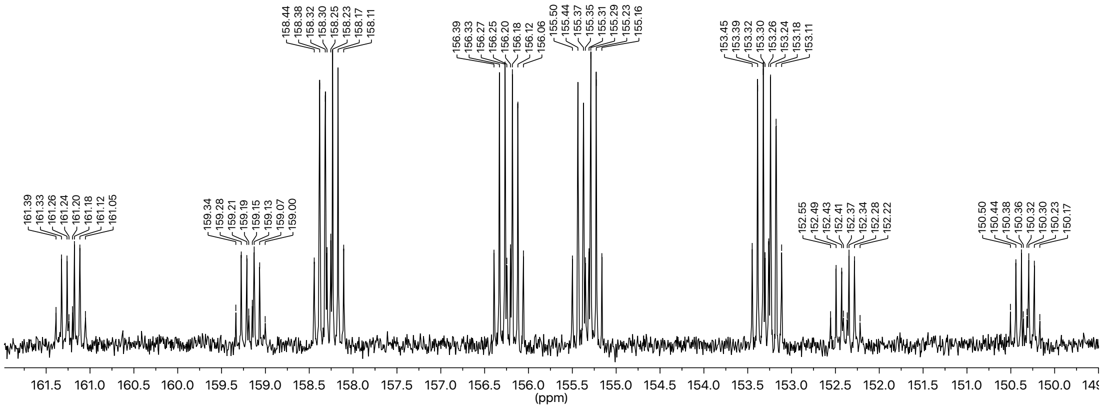
NMR characterization of 8_{NBu_4}

^{1}H NMR spectrum of $\mathbf{8}_{NBu_4}$ at 25 ºC (DMF-d$_7$)

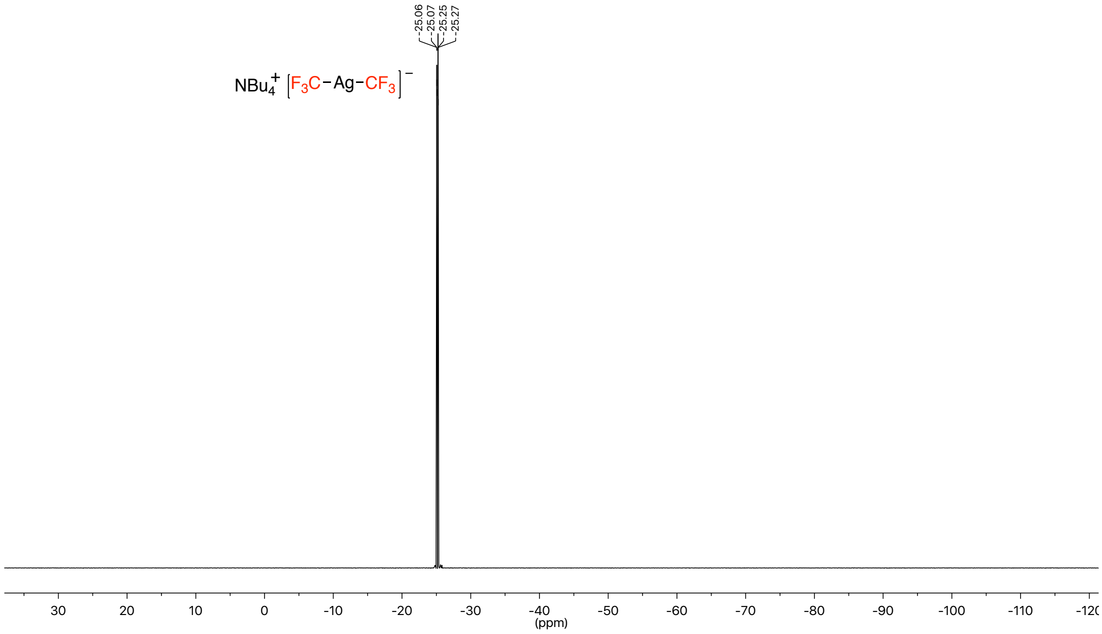


^{13}C NMR spectrum of $\mathbf{8}_{NBu_4}$ at 25 ºC (DMF-d$_7$)





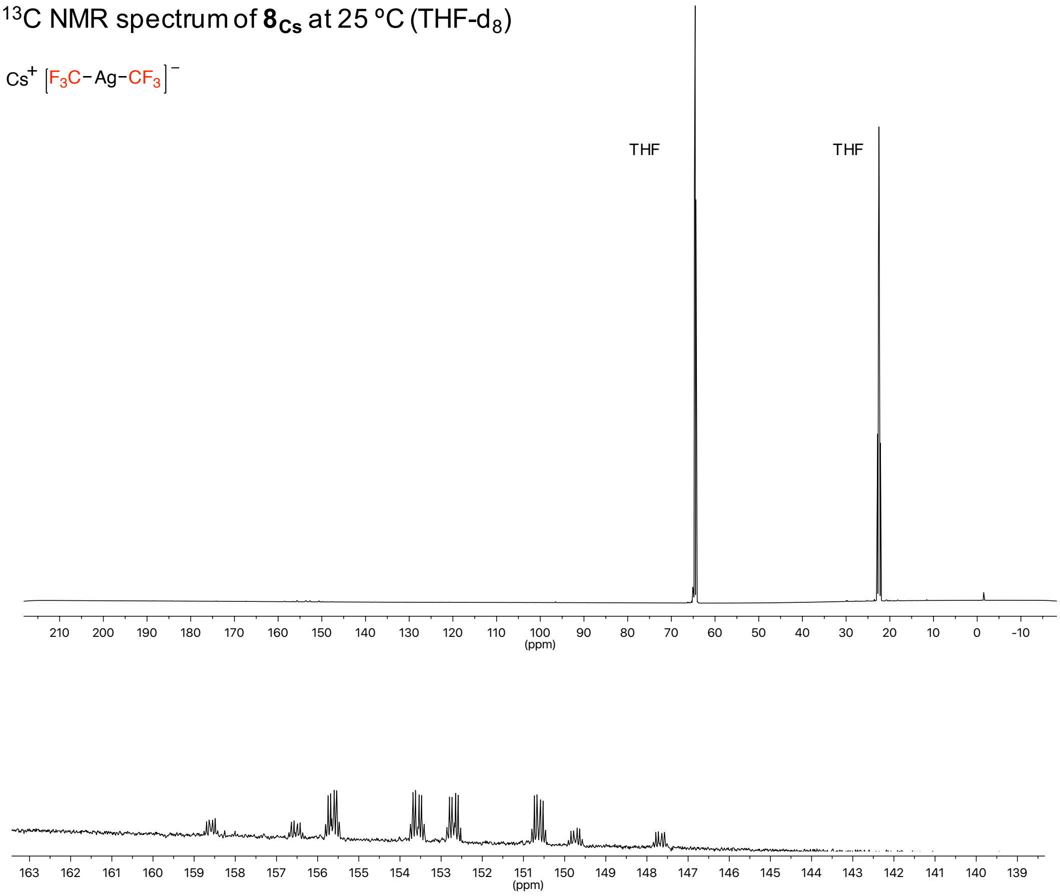
^{19}F NMR spectrum of $\mathbf{8_{NBu_4}}$ at 25 ºC (DMF-d$_7$)



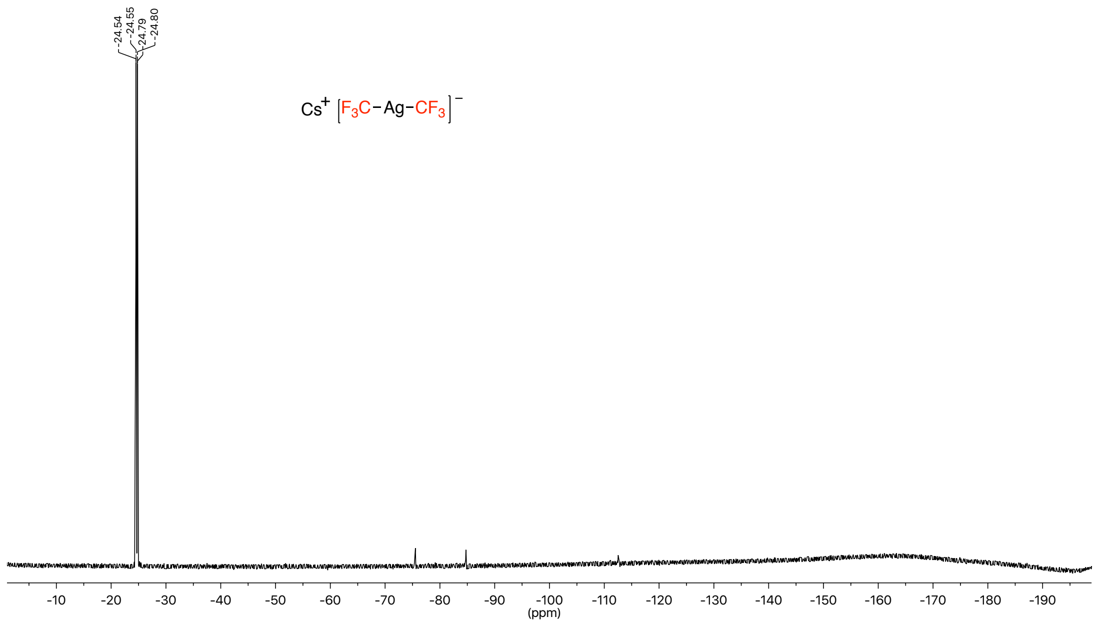
NMR characterization of 8_{Cs}

^{13}C NMR spectrum of $\mathbf{8_{Cs}}$ at 25 ºC (THF-d_8)

$Cs^+ [F_3C–Ag–CF_3]^-$



^{19}F NMR spectrum of $\mathbf{8_{Cs}}$ at 25 ºC (THF-d_8)



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