Copper(I) and silver(I) chemistry of vinyltrifluoroborate supported by a bis(pyrazolyl)methane

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Supporting Information

Table S1. NMR spectroscopic data of vinyltrifluoroborates in $CDCl_3$

compound	^{1}H NMR δ (ppm)	^{13}C NMR δ (ppm)	^{19}F NMR δ (ppm)	^{11}B NMR δ (ppm)	Ref.
(SIPr)Cu(MeCN)(CH_2=$CHBF_3$)	5.06 (m) 4.66 (d) 4.36 (m)	99.9	-149.5 (br.s)	-1.16 (q)	This work
(SIPr)Ag(CH_2=$CHBF_3$)	5.91 (m) 5.27 (dd) 5.10 (br d)	114.3	-143.1 (m)		1
[CH_2(3,5-(CH_3)$_2$Pz)$_2$]Cu(CH_2=$CHBF_3$)	5.32 (m) 4.83 (d) 4.61 (br d)	87.3	-140.1 (br.s)	-0.92 (br s)	This work
[CH_2(3,5-(CH_3)$_2$Pz)$_2$]Ag(CH_2=$CHBF_3$)	6.15 (m) 5.59 (dd) 5.31 (m)	102.2	-142.0 (br s)	-1.24 (br s)	This work

Figure S1. ^{1}H NMR of (SIPr)Cu(MeCN)(CH_2=$CHBF_3$) **(4)**

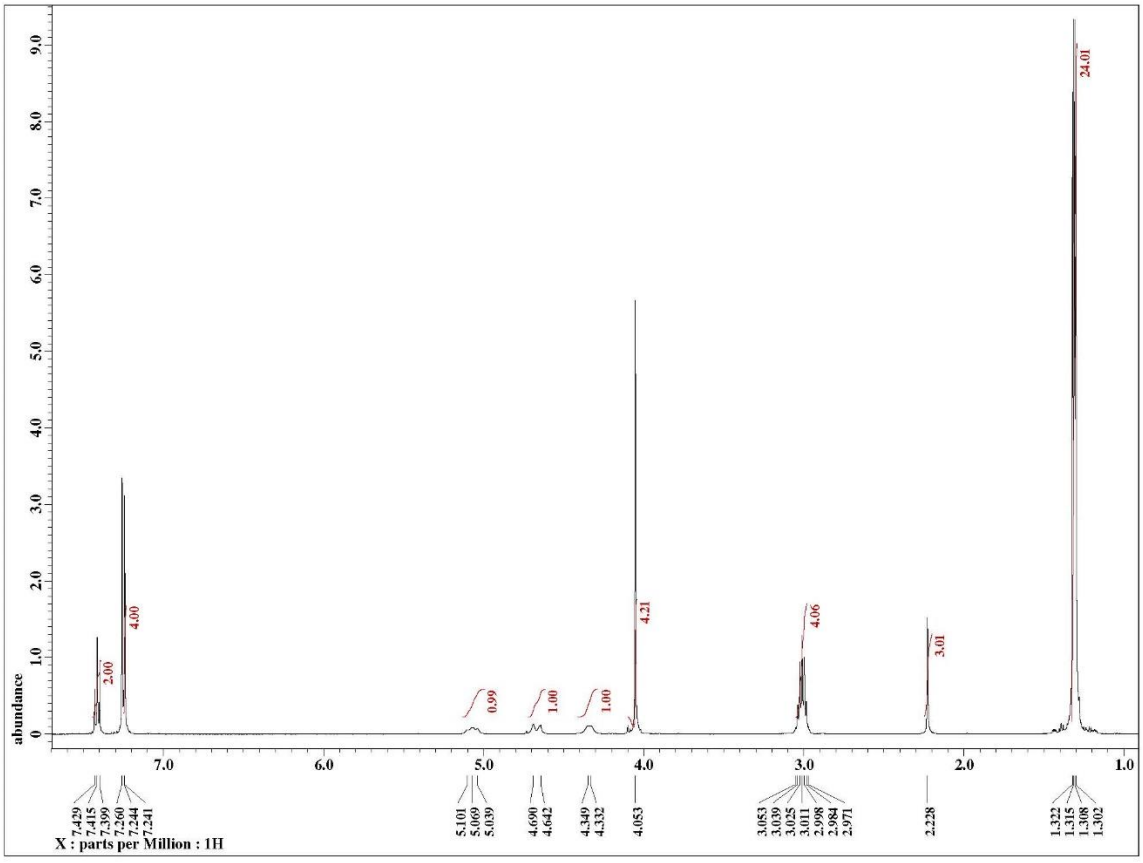


Figure S2. ^{1}H NMR (zoomed) of (SIPr)Cu(MeCN)(CH_2=$CHBF_3$) **(4)**

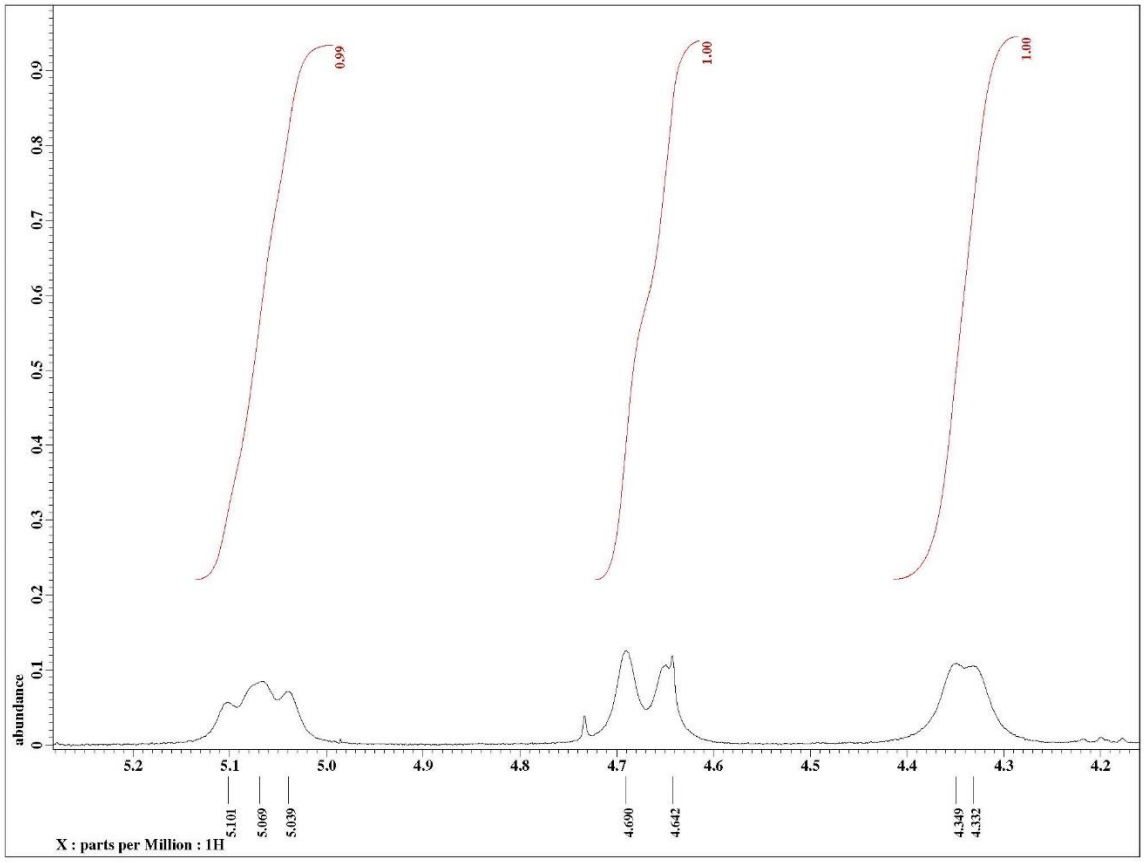


Figure S3. ^{1}H NMR (zoomed) of (SIPr)Cu(MeCN)(CH_2=$CHBF_3$) **(4)**

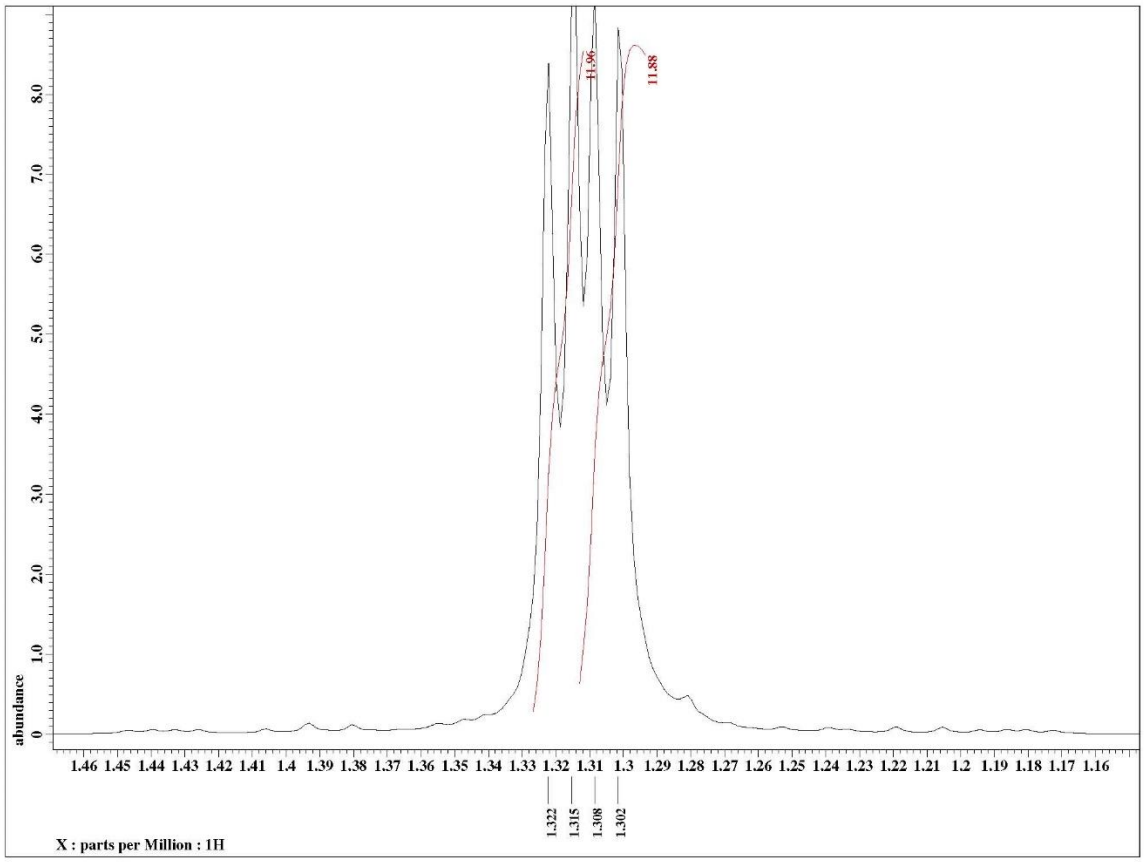


Figure S4. ^{19}F NMR of (SIPr)Cu(MeCN)(CH_2=$CHBF_3$) **(4)**

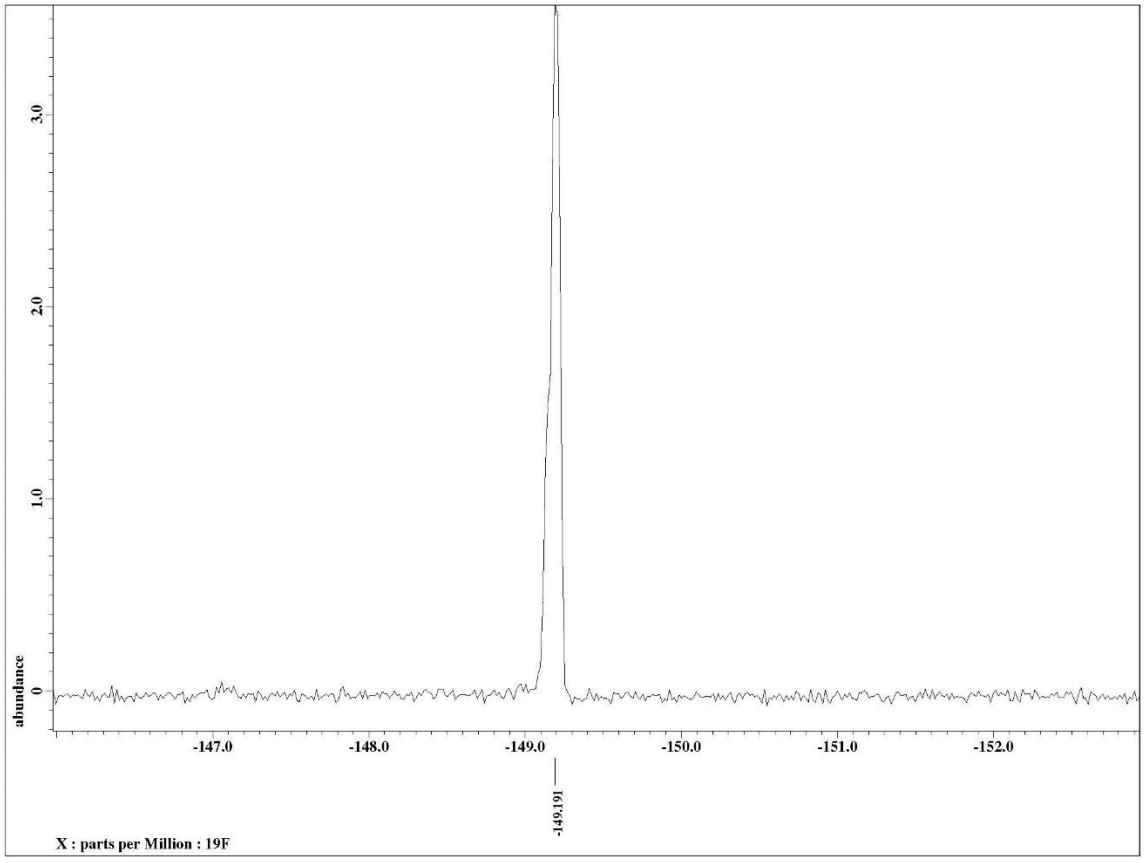


Figure S5. ^{13}C NMR of (SIPr)Cu(MeCN)(CH_2=$CHBF_3$) **(4)**

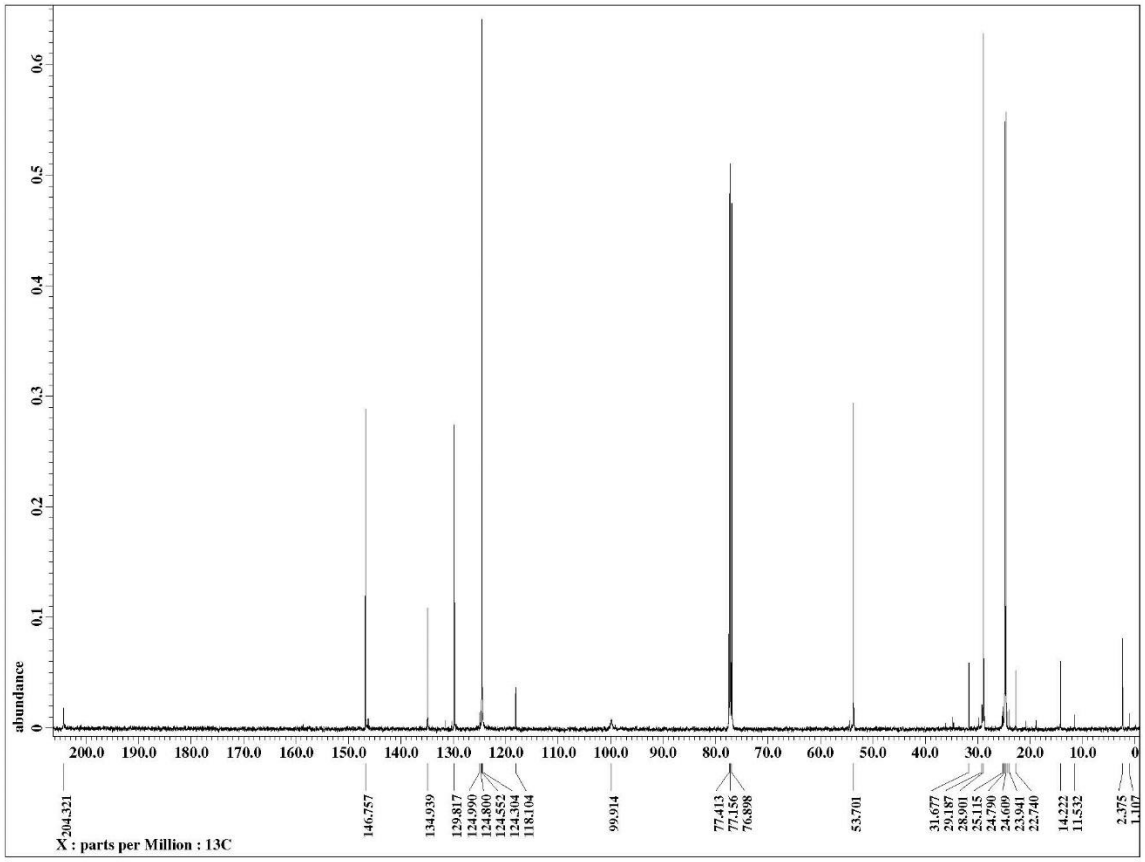
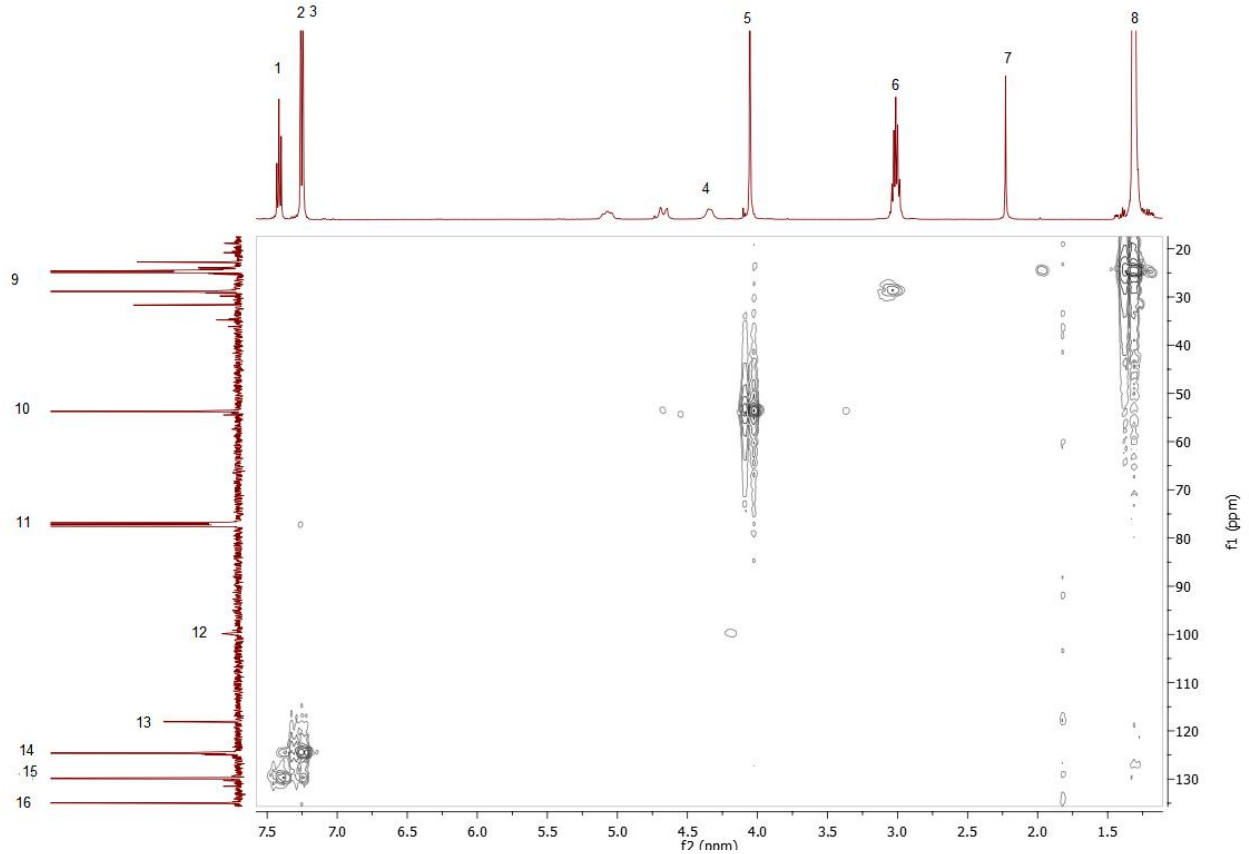


Figure S6. HMQC NMR of (SIPr)Cu(MeCN)(CH_2=$CHBF_3$) **(4)**



^{1}H NMR (in $CDCl_3$): δ (ppm) 7.43 (CH_{Ar}), 7.26 (CH_{Ar}), 5.06 (CH_2CHBF_3), 4.66 (CH_2CHBF_3), 4.36 (CH_2CHBF_3), 4.05 (NCH_2), 3.02 ($CH(CH_3)_2$), 2.23 (CH_3CN), 1.32 (CH_3), 1.31 (CH_3).

^{13}C{^{1}H} NMR (in $CDCl_3$): δ (ppm) 134.0(CH_{Ar}), 129.8 (CH_{Ar}), 124.5 (CH_{Ar}), 118.1, 99.9 (*C*H_2CHBF_3), 53.7 (N*C*H_2), 31.7-24.7 ($CH(CH_3)_2$).

In the HMQC spectrum, ^{1}H signals #1 (7.43 ppm (CH_{Ar})) corresponds to #15 (129.8 ppm (CH_{Ar}), #2 corresponds to solvent peak #11, #3 (7.26 ppm (CH_{Ar}) corresponds to #14 (124.5 ppm (CH_{Ar})), #4 (4.36 ppm (CH_2CHBF_3)) corresponds to #12 (99.9 ppm, (CH_2CHBF_3)), #5 (4.07 ppm (NCH_2)) corresponds to #10 (53.7 ppm (NCH_2)), #6 (3.02 ppm ($CH(CH_3)_2$) corresponds to #9 (31.7-24.7 ppm $CH(CH_3)_2$) and #8 (1.33-1.32 ppm (CH_3)) corresponds to #9 (31.7-24.7 ppm $CH(CH_3)_2$).

Figure S7. ^{11}B NMR of (SIPr)Cu(MeCN)(CH_2=$CHBF_3$) **(4)**

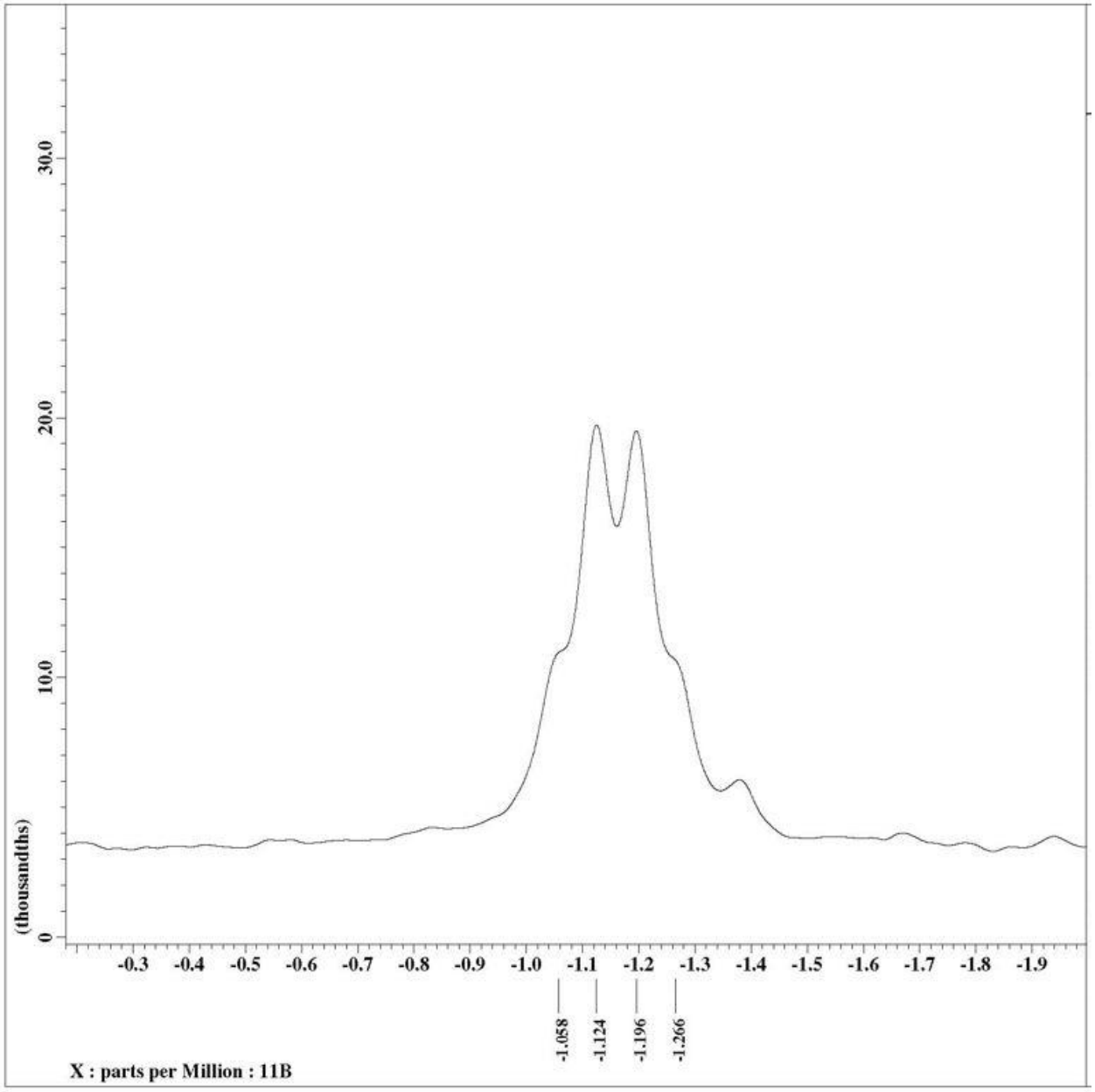


Figure S8. ^{1}H NMR of $(MeCN)_3Cu(CH_2=CHBF_3)$

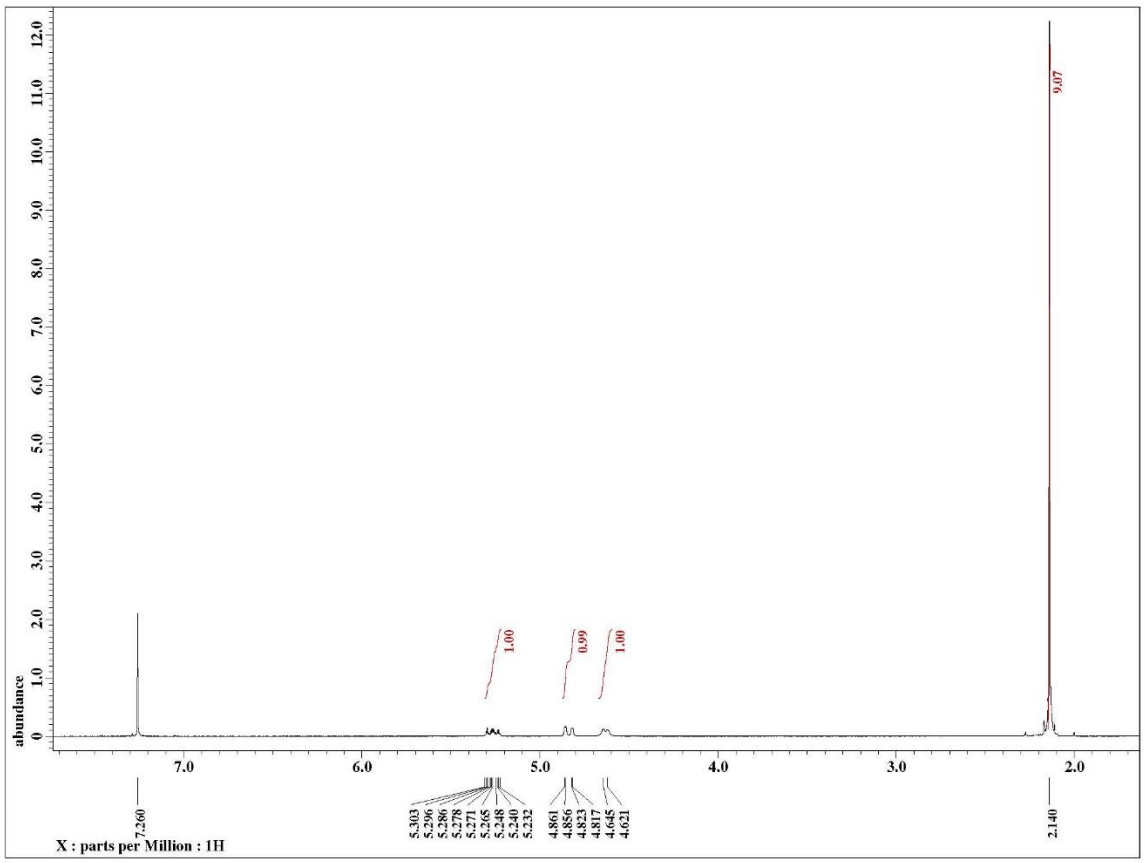


Figure S9. ^{1}H NMR (zoomed) of $(MeCN)_3Cu(CH_2=CHBF_3)$

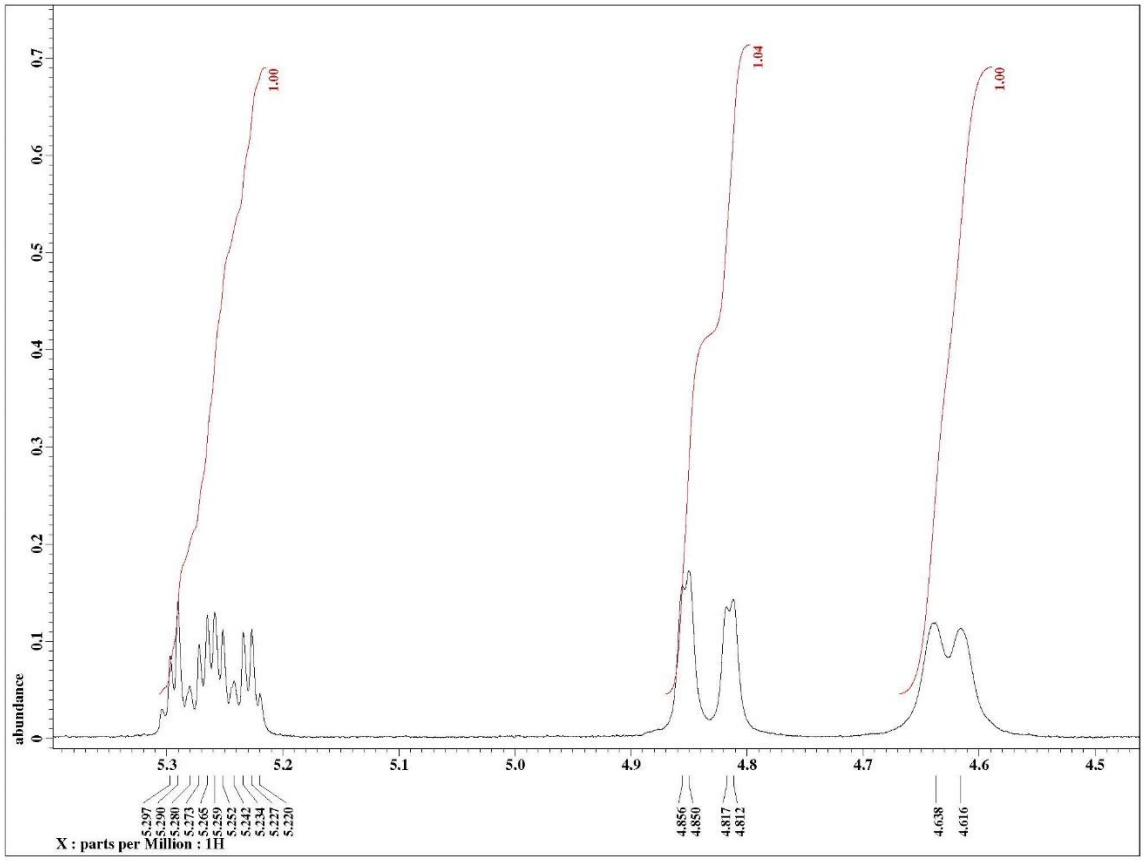


Figure S10. ^{19}F NMR of $(MeCN)_3Cu(CH_2=CHBF_3)$

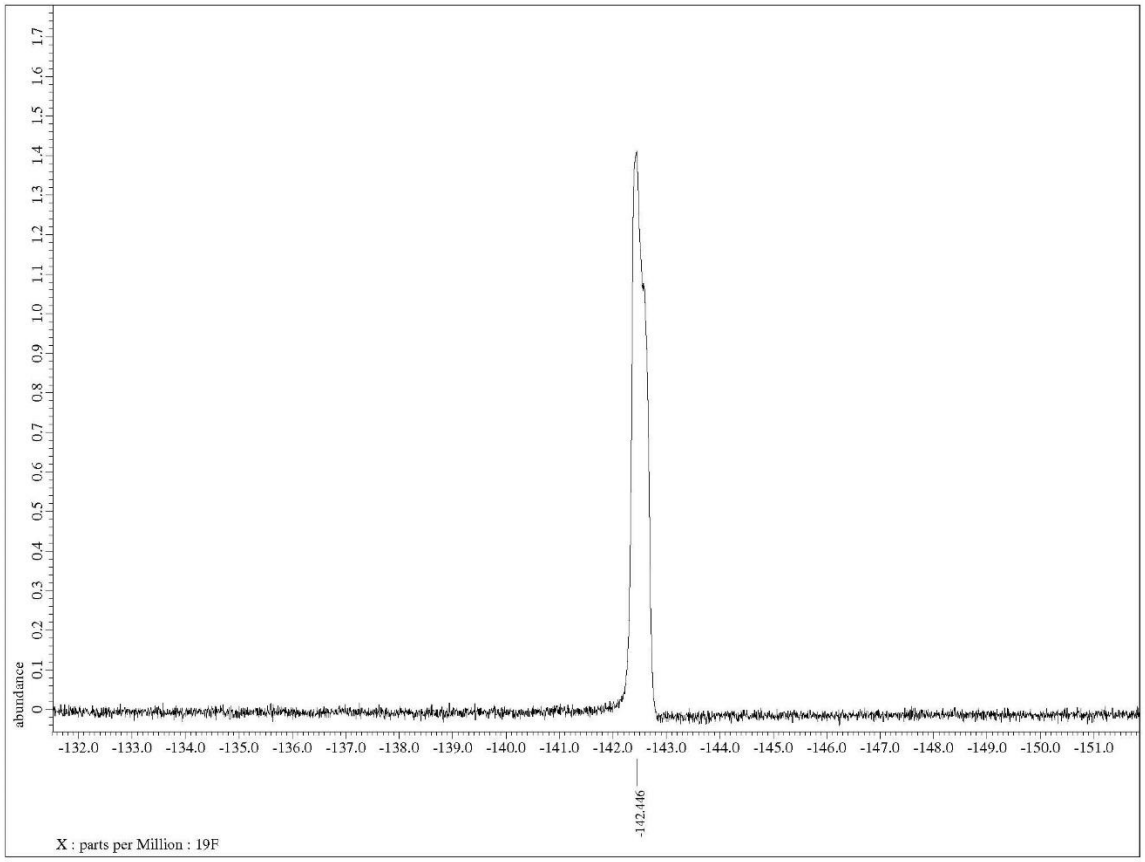


Figure S11. ^{13}C NMR of $(MeCN)_3Cu(CH_2=CHBF_3)$

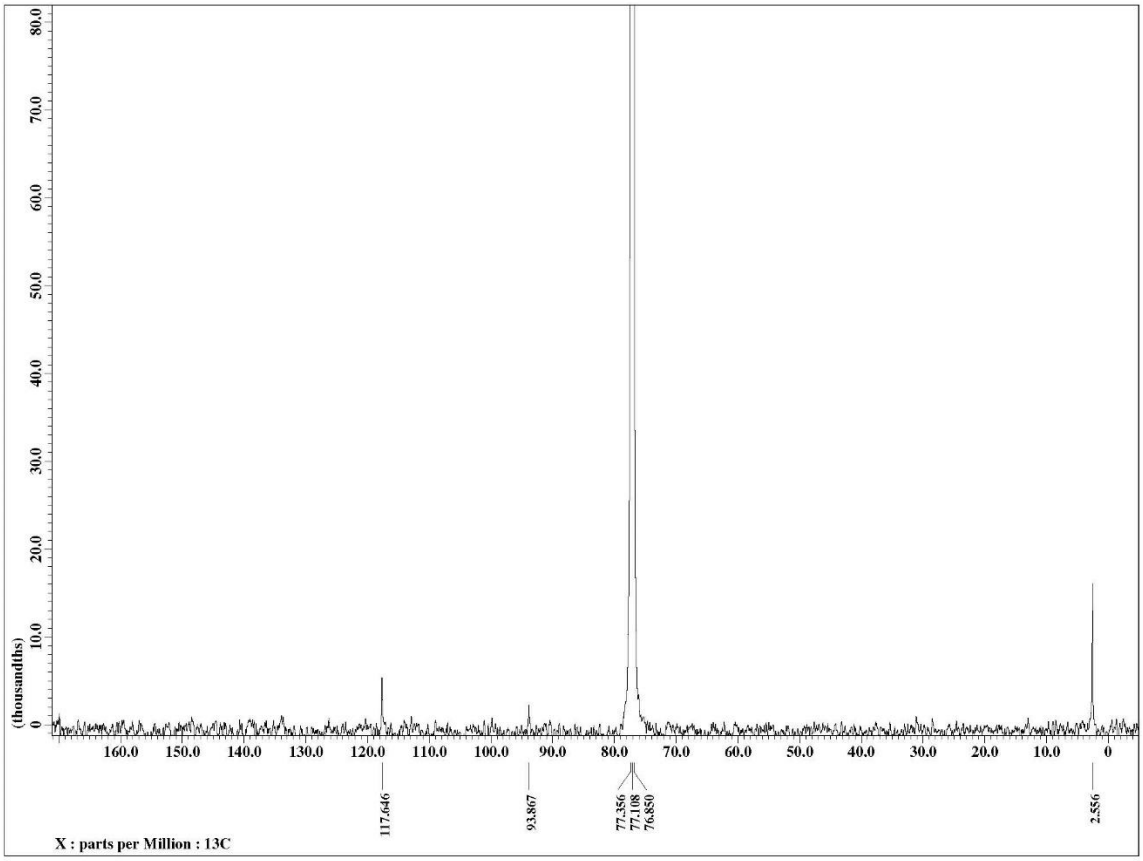


Figure S12. ^{1}H NMR of $[CH_2(3,5\text{-}(CH_3)_2Pz)_2]Cu(CH_2{=}CHBF_3)$ **(5)**

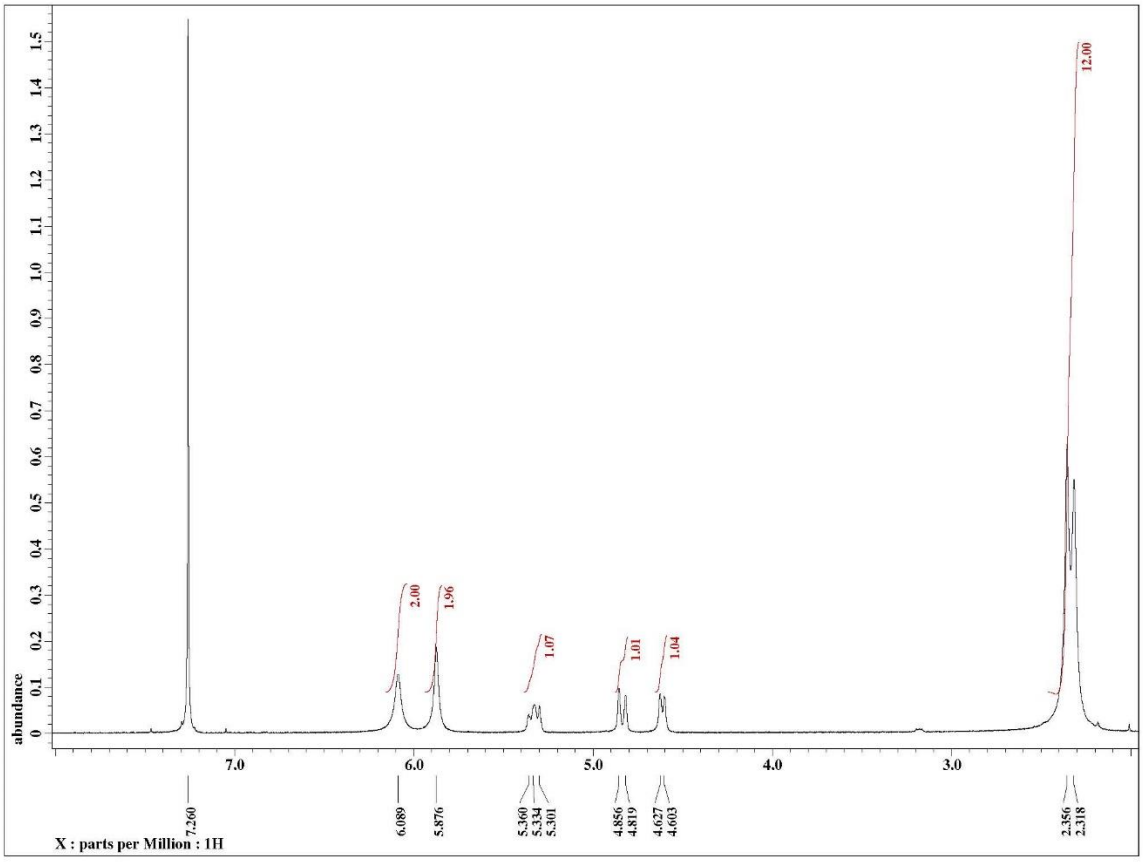


Figure S13. ^{1}H NMR (zoomed) $[CH_2(3,5\text{-}(CH_3)_2Pz)_2]Cu(CH_2{=}CHBF_3)$ **(5)**

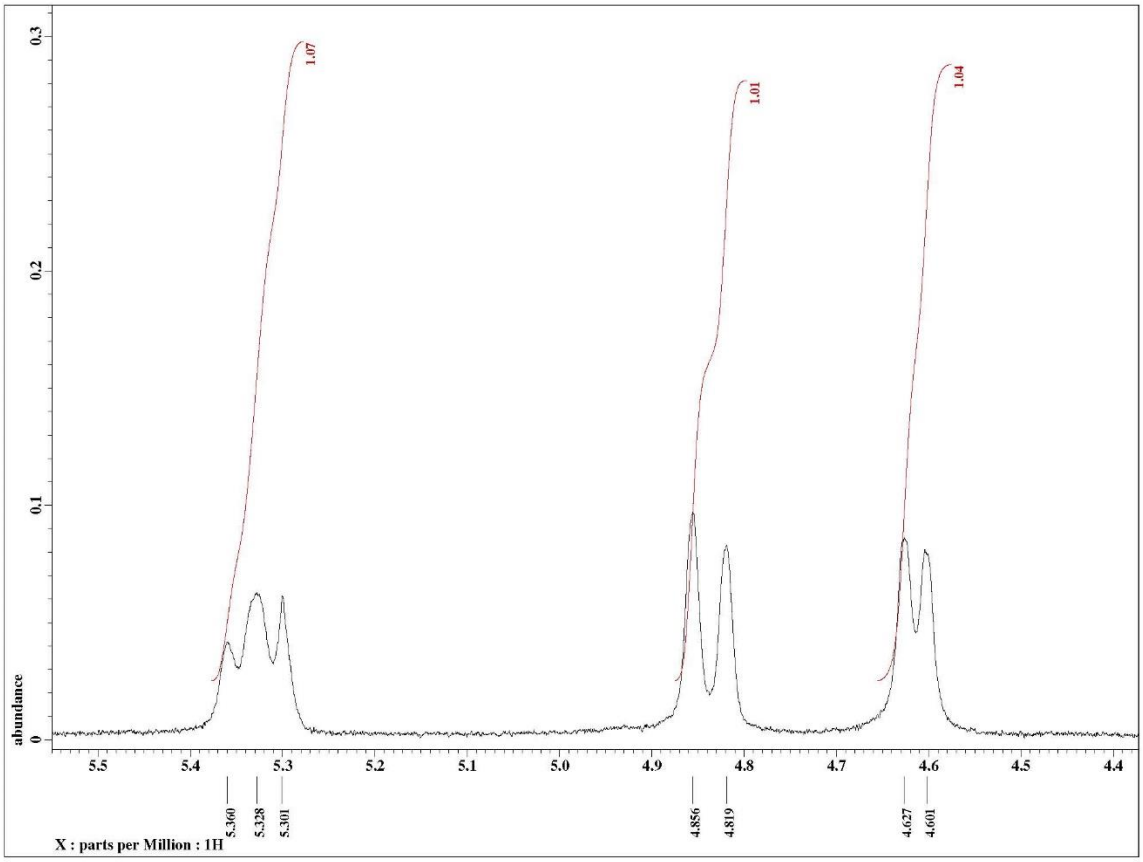


Figure S14. ^{19}F NMR of $[CH_2(3,5\text{-}(CH_3)_2Pz)_2]Cu(CH_2{=}CHBF_3)$ **(5)**

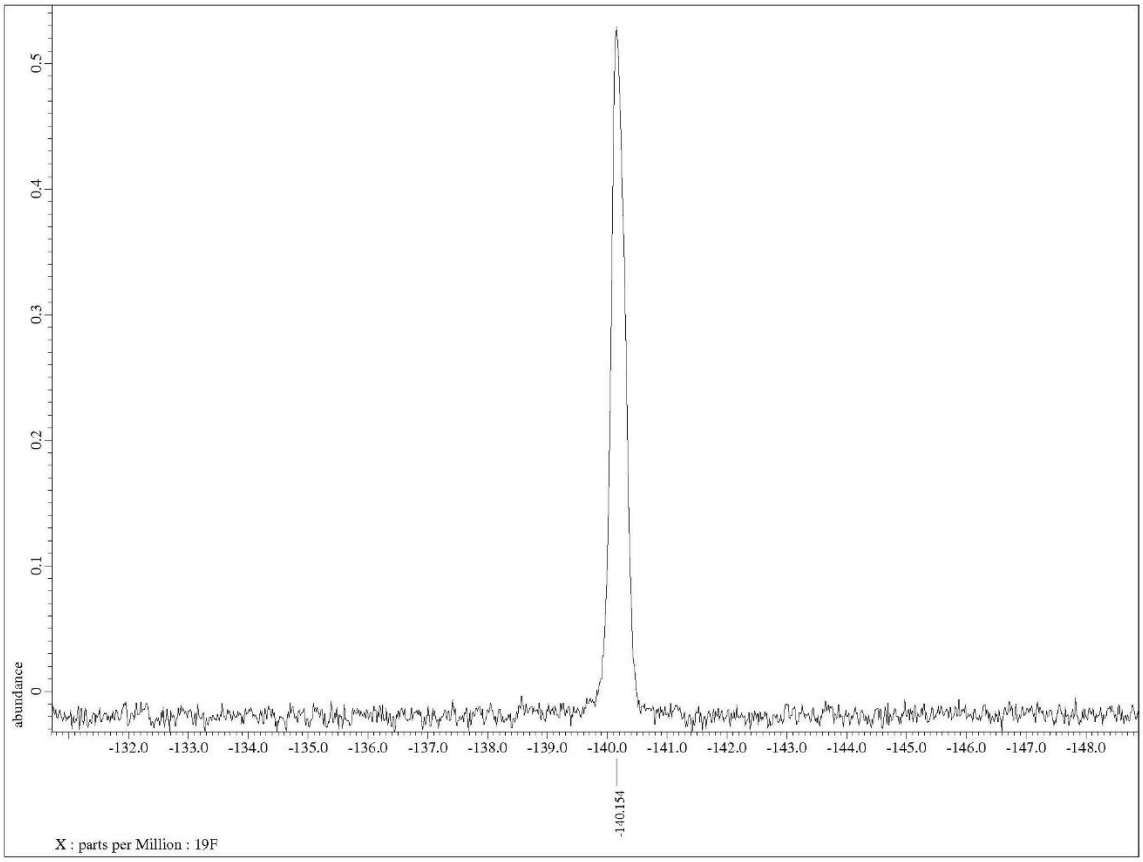


Figure S15. ^{13}C NMR of $[CH_2(3,5\text{-}(CH_3)_2Pz)_2]Cu(CH_2{=}CHBF_3)$ **(5)**

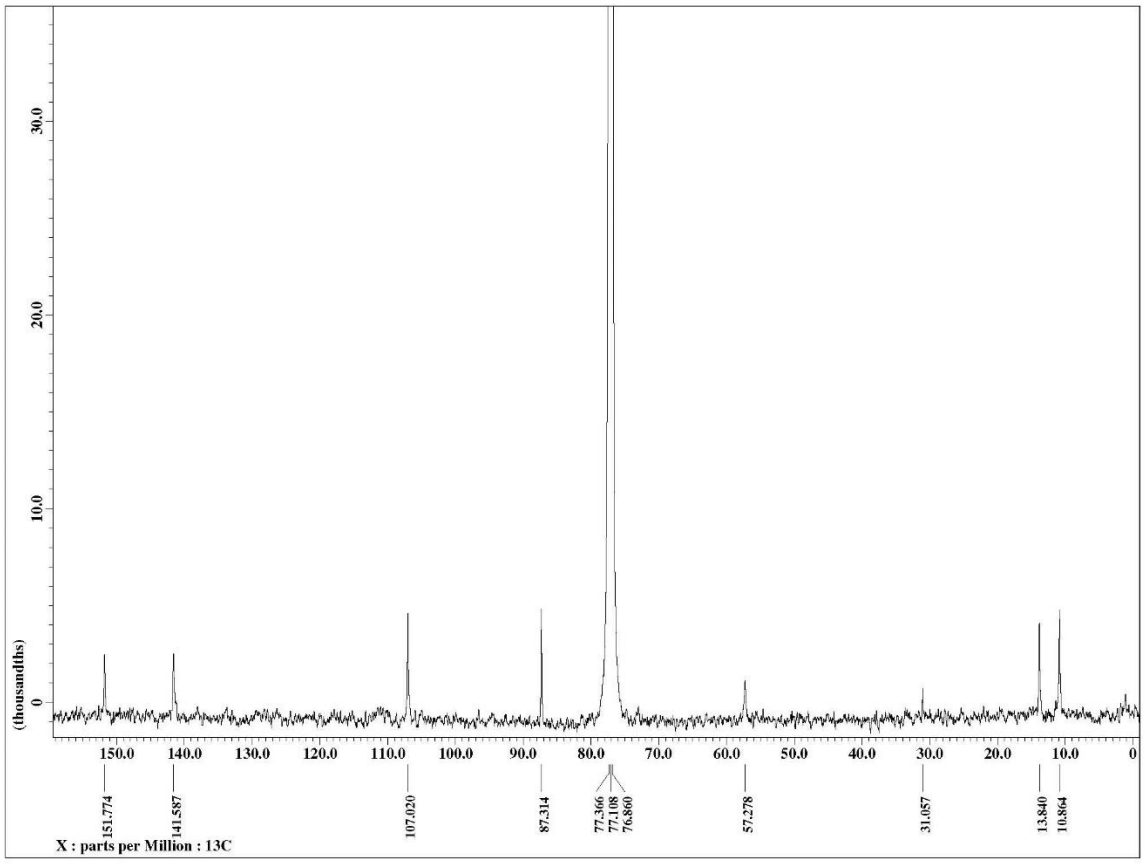


Figure S16. ^{11}B NMR of $[CH_2(3,5\text{-}(CH_3)_2Pz)_2]Cu(CH_2{=}CHBF_3)$ **(5)**

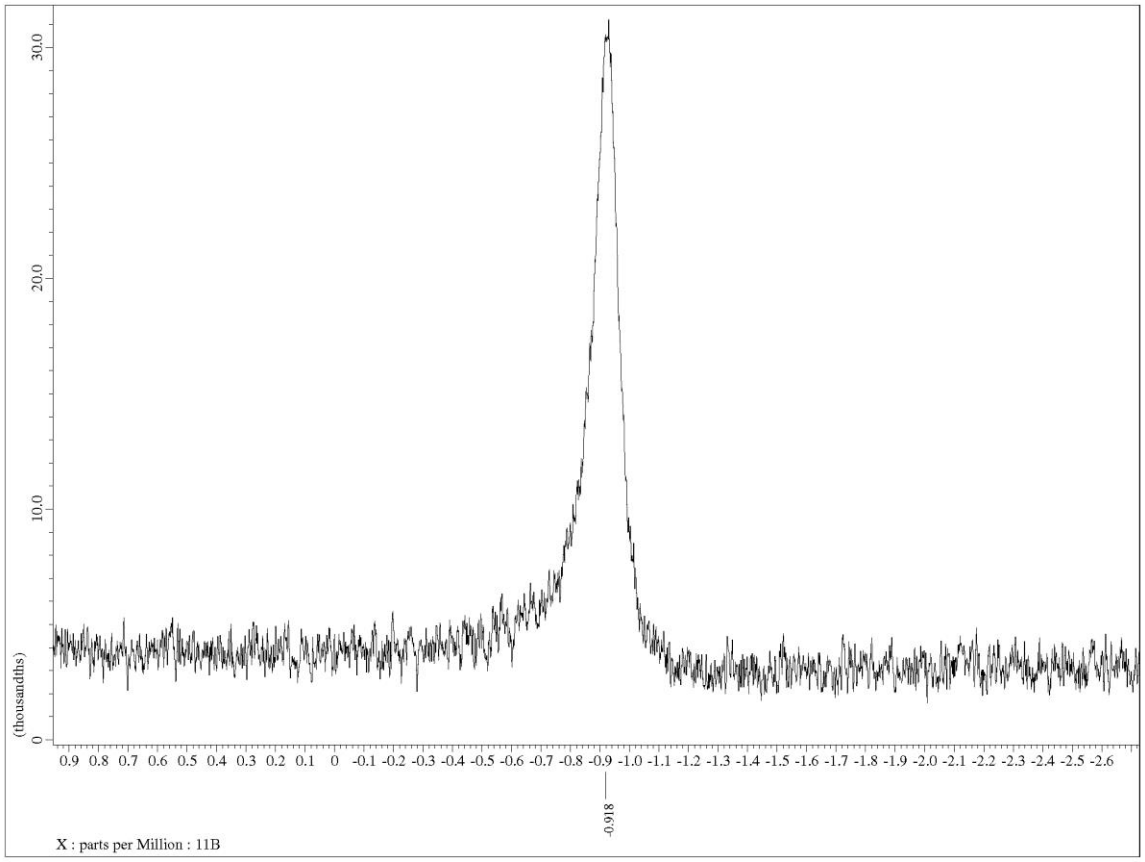


Figure S17. IR of $K(CH_2=CHBF_3)$

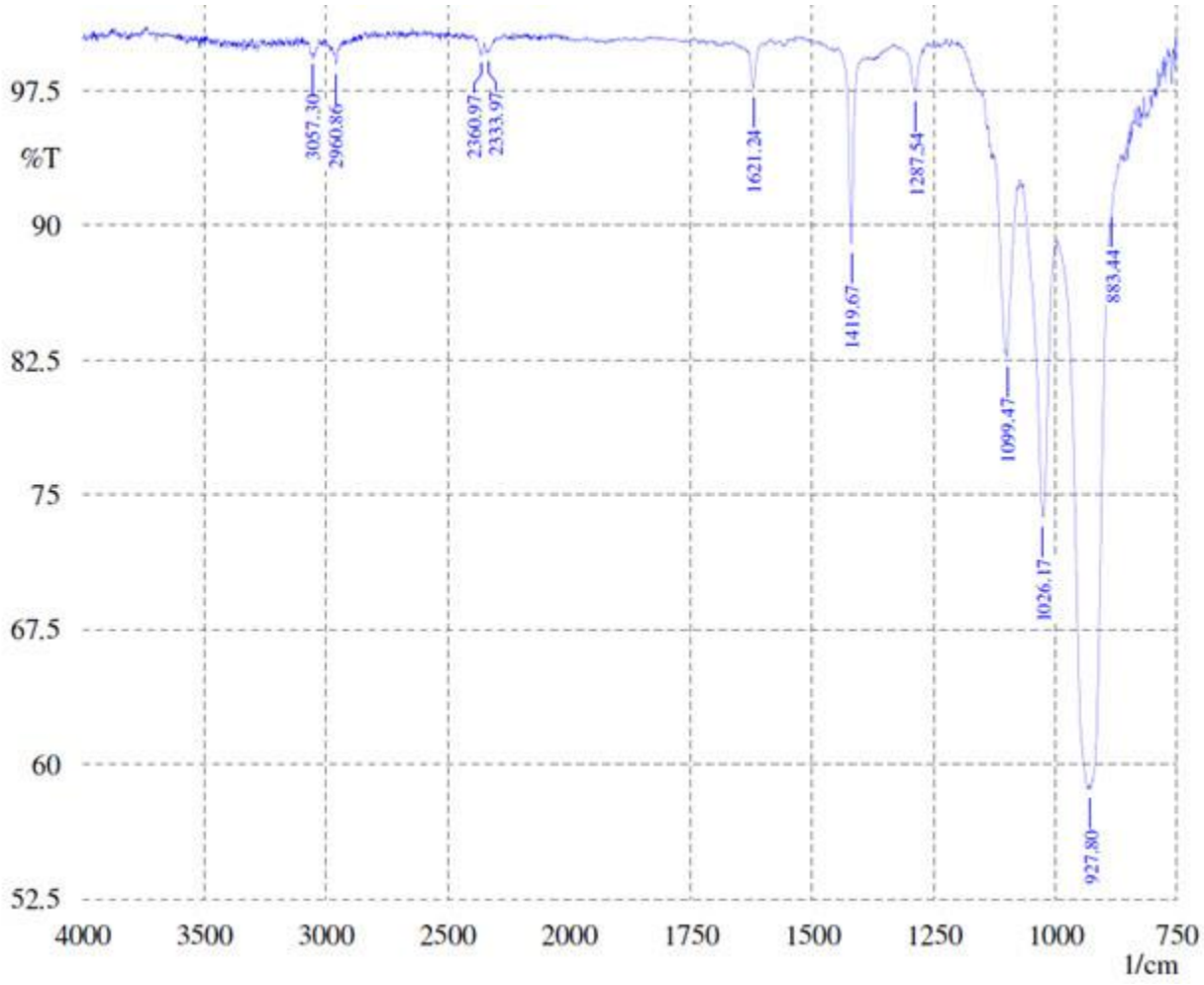


Figure S18. IR of $[CH_2(3,5\text{-}(CH_3)_2Pz)_2]Cu(CH_2{=}CHBF_3)$ **(5)**

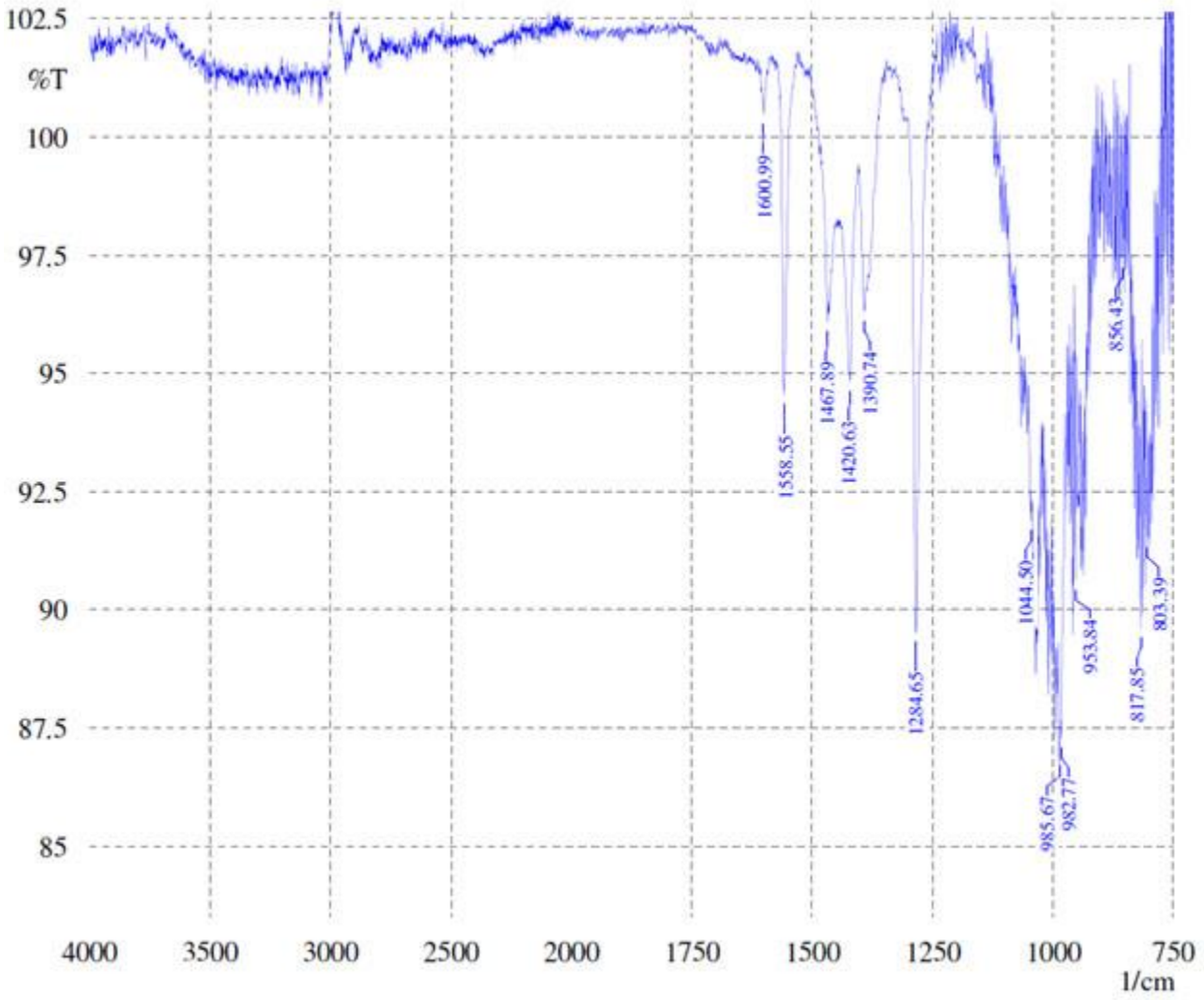


Figure S19. ^{1}H NMR of $(MeCN)_3Ag(CH_2=CHBF_3)$

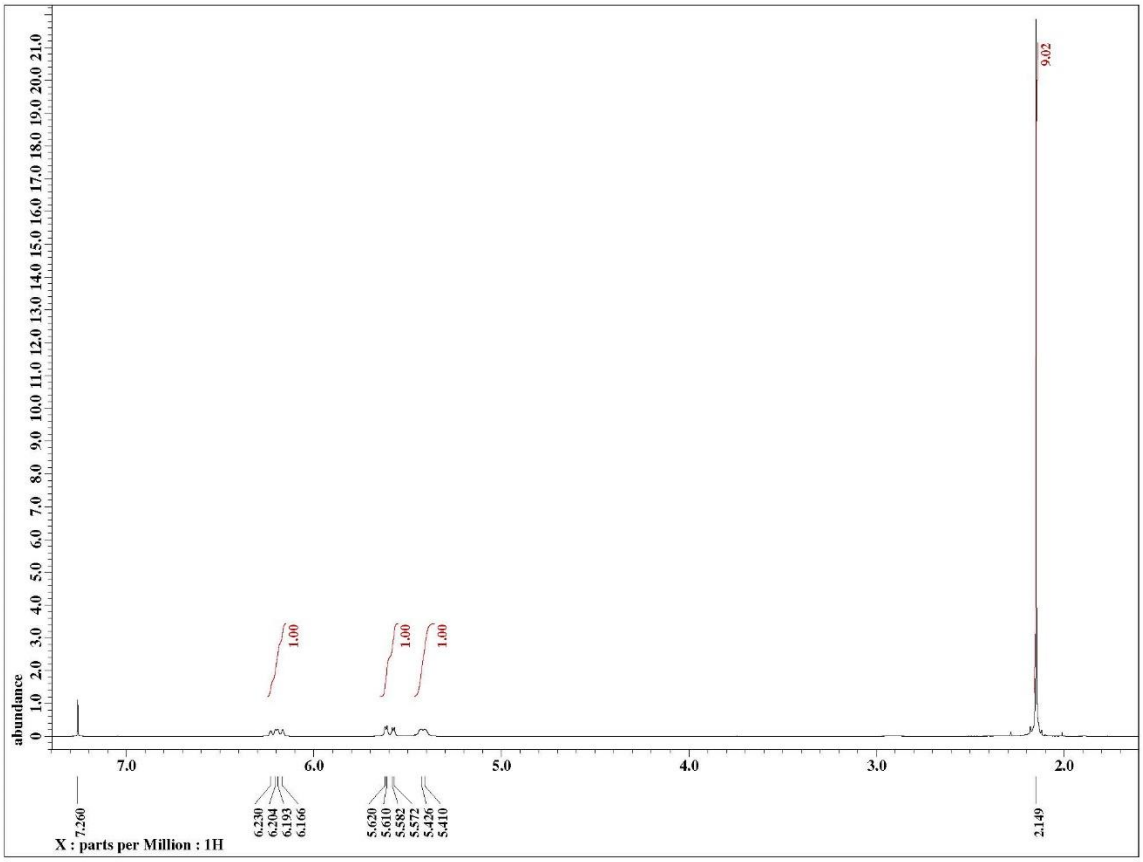


Figure S20. ^{1}H NMR (zoomed) of $(MeCN)_3Ag(CH_2=CHBF_3)$

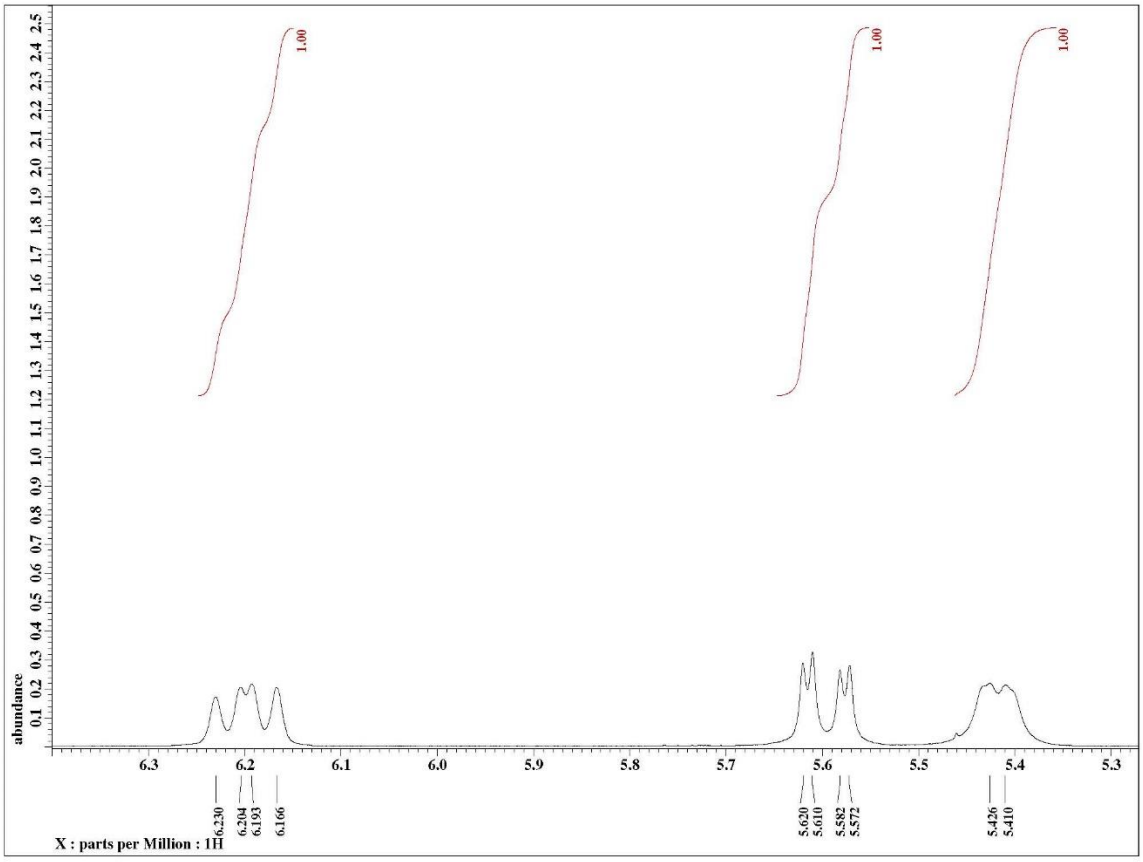


Figure S21. ^{19}F NMR of $(MeCN)_3Ag(CH_2=CHBF_3)$

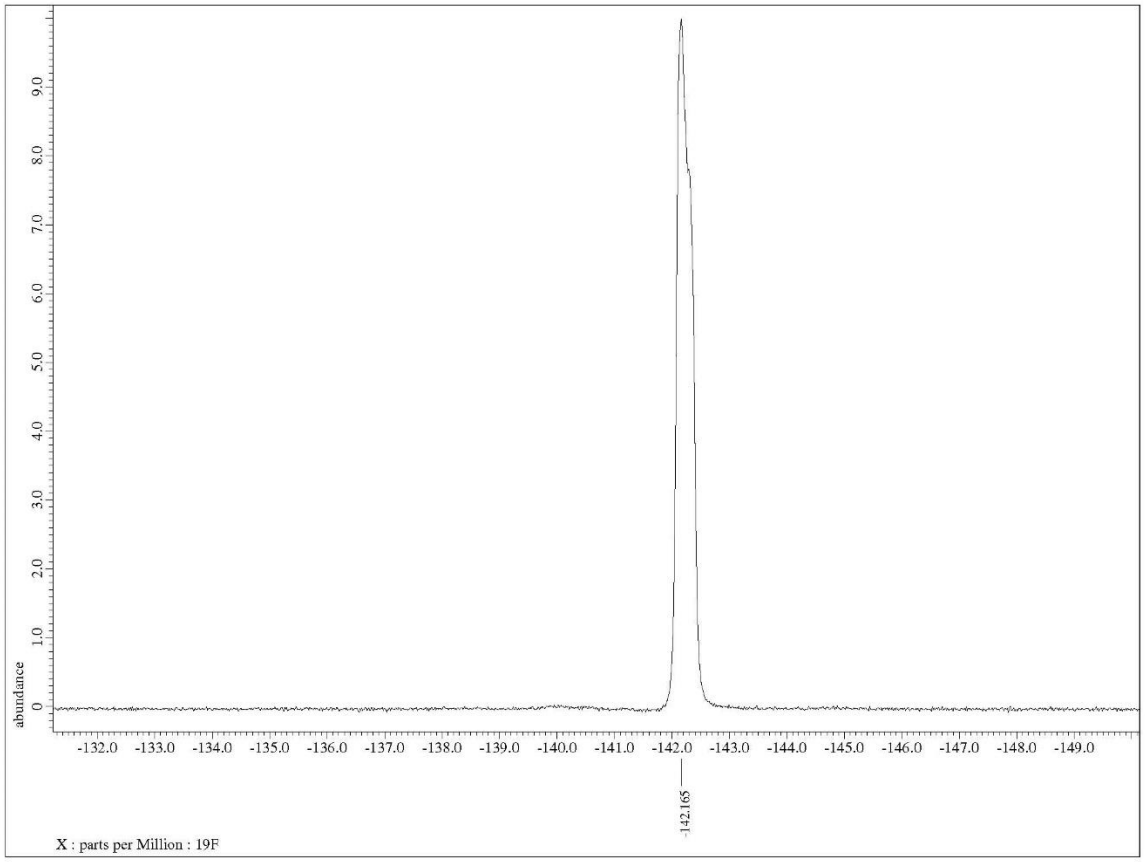


Figure S22. ^{13}C NMR of $(MeCN)_3Ag(CH_2=CHBF_3)$

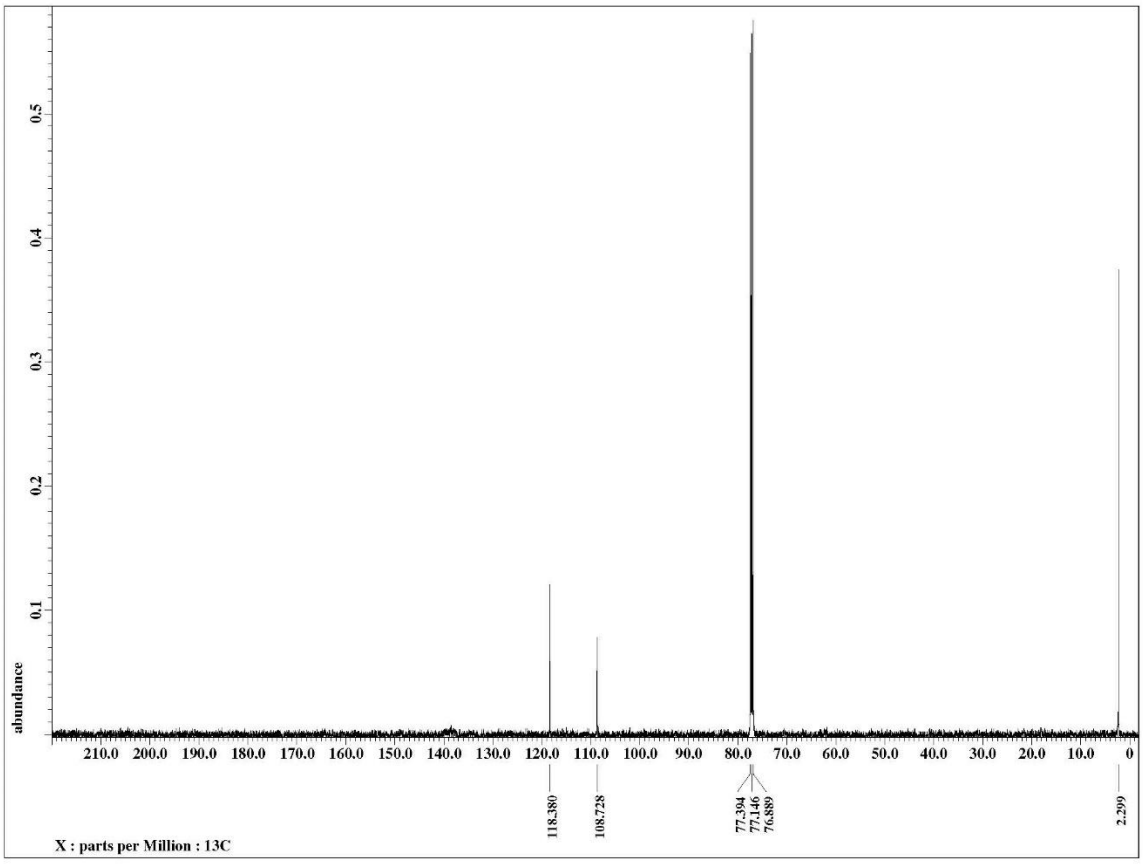


Figure S23. ^{1}H NMR of $[CH_2(3,5\text{-}(CH_3)_2Pz)_2]Ag(CH_2{=}CHBF_3)$ **(6)**

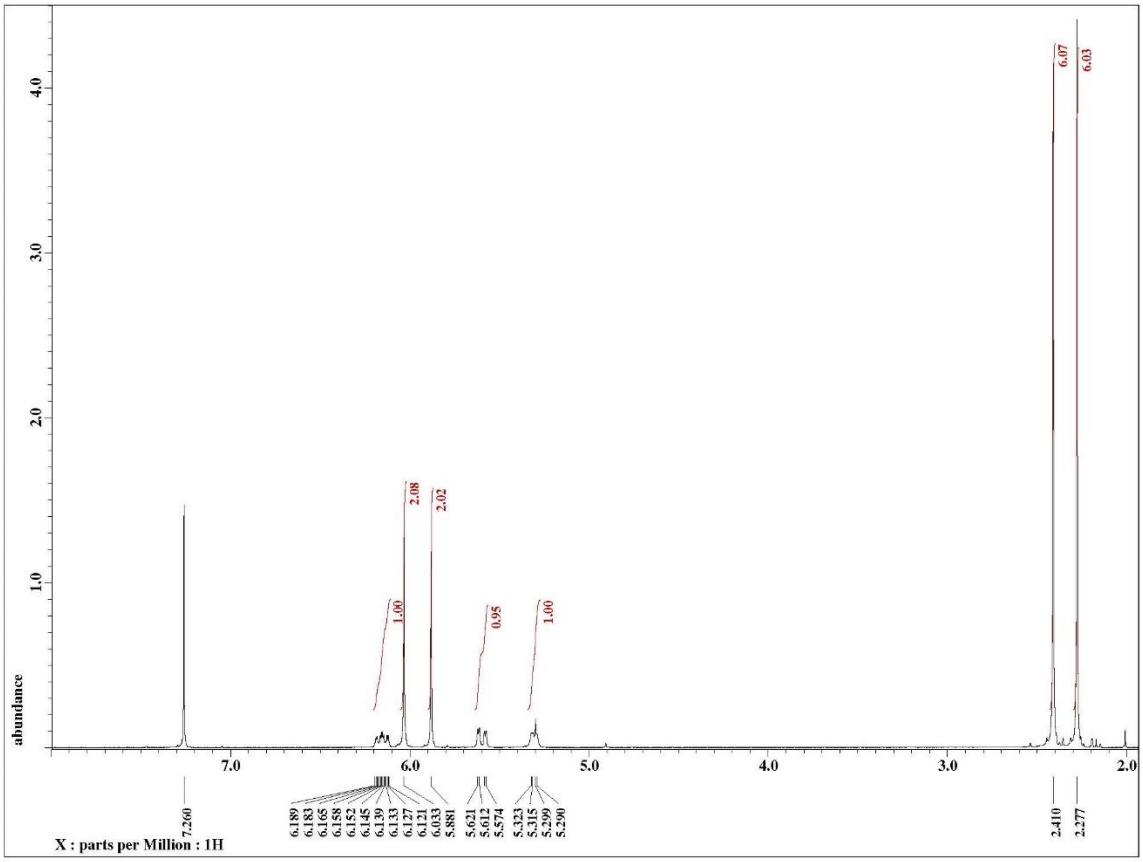


Figure S24. ^{1}H NMR (zoomed) of $[CH_2(3,5\text{-}(CH_3)_2Pz)_2]Ag(CH_2{=}CHBF_3)$ **(6)**

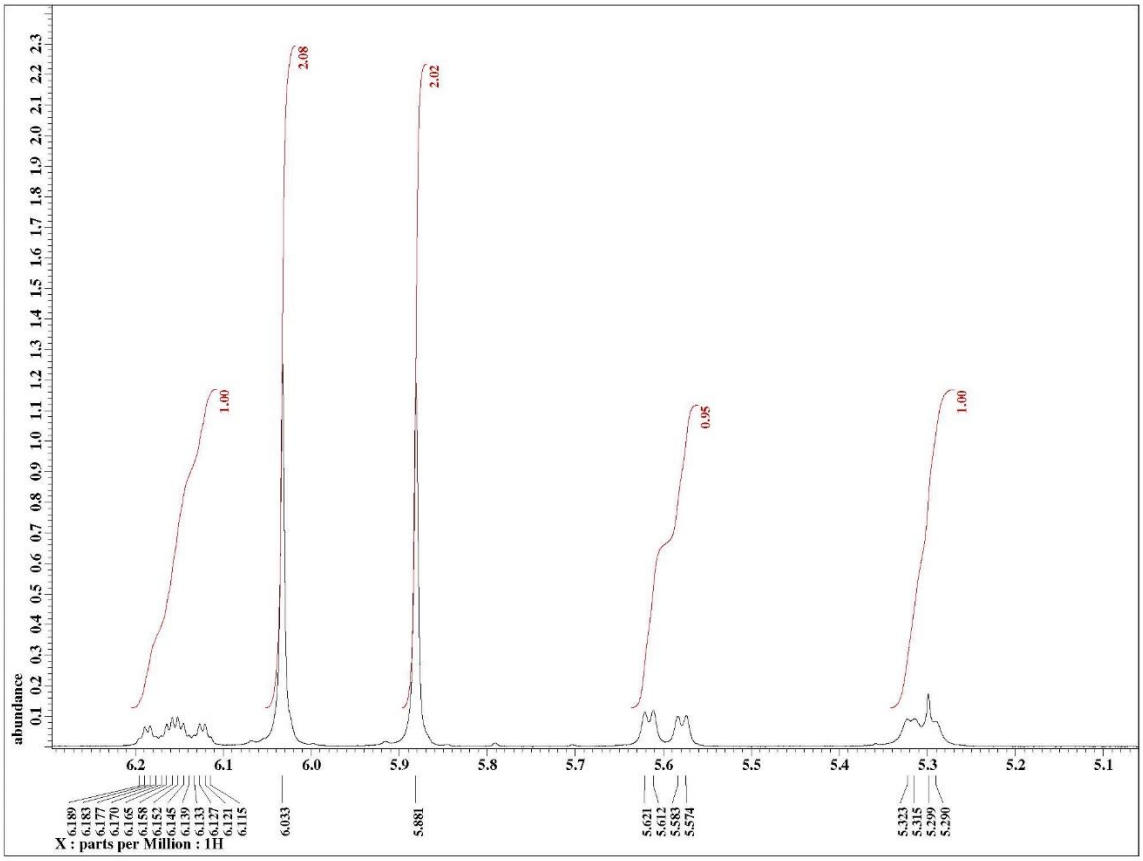


Figure S25. ^{19}F NMR of $[CH_2(3,5\text{-}(CH_3)_2Pz)_2]Ag(CH_2{=}CHBF_3)$ **(6)**

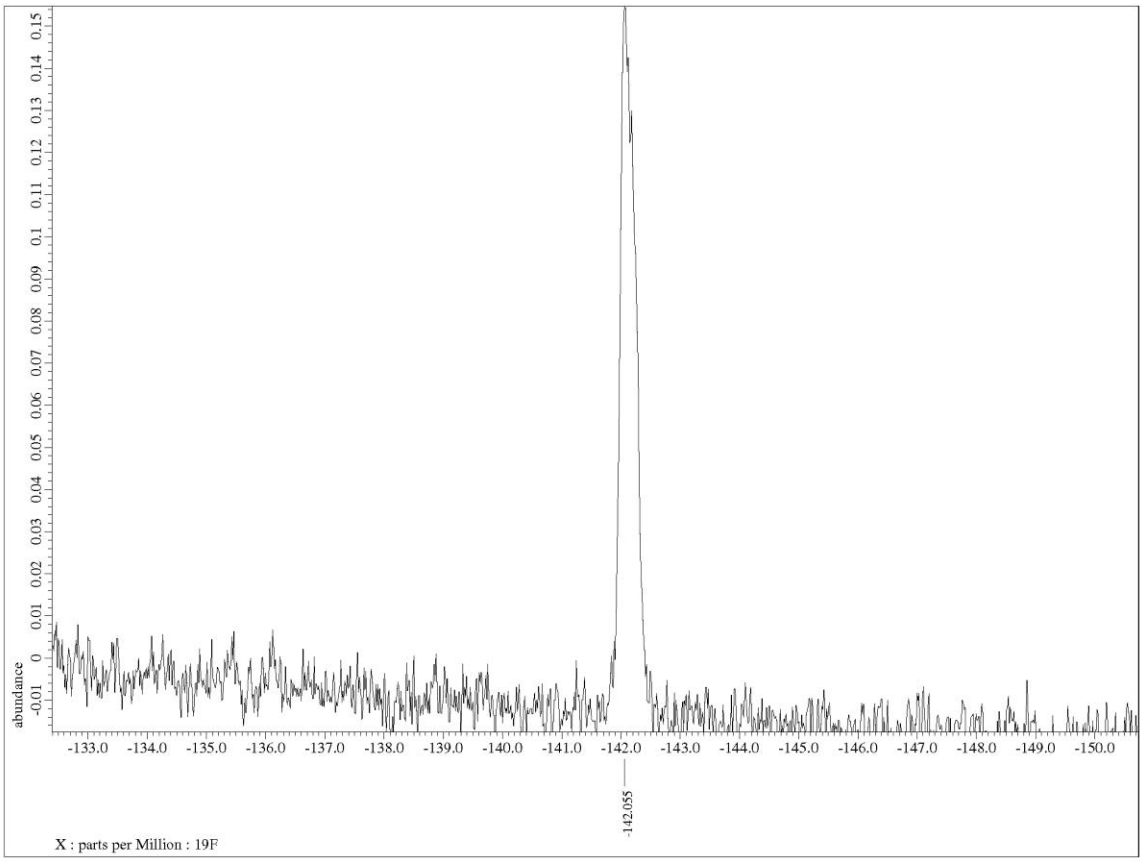


Figure S26. ^{13}C NMR of $[CH_2(3,5\text{-}(CH_3)_2Pz)_2]Ag(CH_2{=}CHBF_3)$ **(6)**

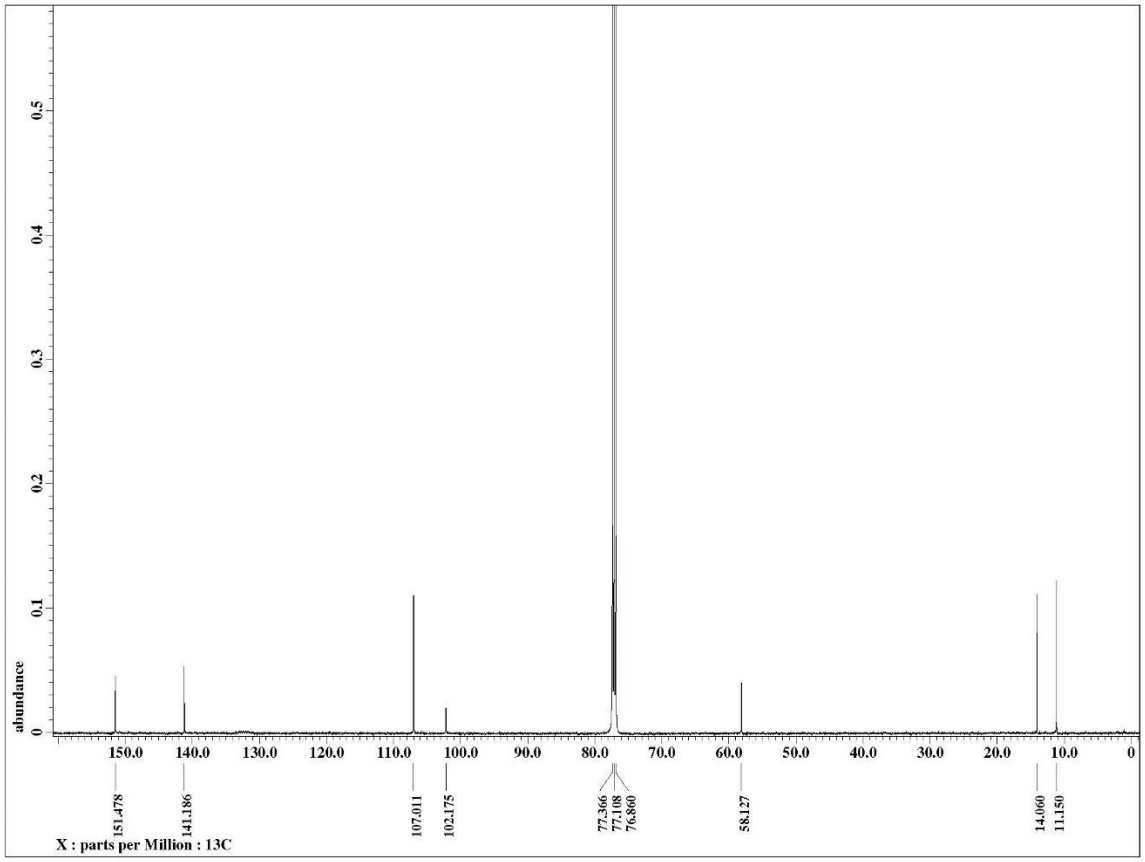
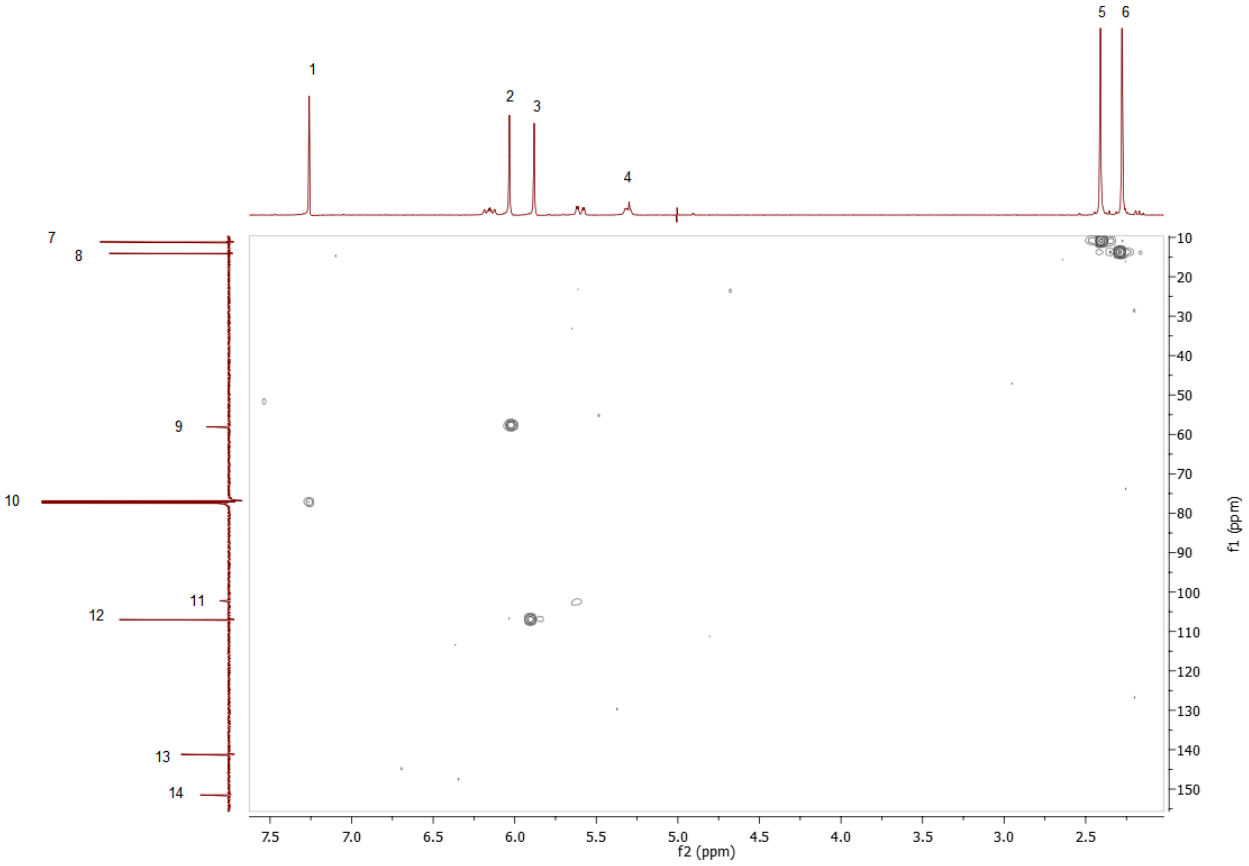


Figure S27. HMQC NMR of $[CH_2(3,5\text{-}(CH_3)_2Pz)_2]Ag(CH_2{=}CHBF_3)$ **(6)**



^{1}H NMR (in $CDCl_3$): δ (ppm) 6.15 (CH_2CHBF_3), 6.03 ($N(CH_2)N$), 5.88 (CH_{Pz}), 5.59 (CH_2CHBF_3), 5.31 (CH_2CHBF_3), 2.41 (CH_3), 2.28 (CH_3) ppm.

$^{13}C\{^1H\}$ NMR (in $CDCl_3$): δ (ppm) 151.5 (s, $C(CH_3)$), 141.2 (s, $C(CH_3)$), 141.2 ($C(CH_3)$), 107.0 (CH_{Pz}), 102.2 (CH_2CHBF_3), 58.1 (CH_2), 14.1 (CH_3), 11.2 (CH_3).

In the HMQC spectrum, ^{1}H signals #1 is the solvent peak corresponding to #10, #2 (6.03 ppm ($N(CH_2)N$)) corresponds to #9 (58.1 ppm (CH_2)), #3 (5.88 ppm (CH_{Pz})) corresponds to #12 (107 ppm, (CH_{Pz})), #4 (5.31 ppm (CH_2CHBF_3)) corresponds to #11 (102.2 ppm (CH_2CHBF_3)), #5 (2.41 ppm (CH_3)) corresponds to #7 (11.2 ppm (CH_3)) and #6 (2.27 ppm (CH_3)) corresponds to #8 (11.2 ppm (CH_3)). There are no proton cross-peaks for # 13 and 14 as these peaks correspond to *C*(CH_3) carbons.

Figure S28. ^{11}B NMR of $[CH_2(3,5\text{-}(CH_3)_2Pz)_2]Ag(CH_2{=}CHBF_3)$ **(6)**

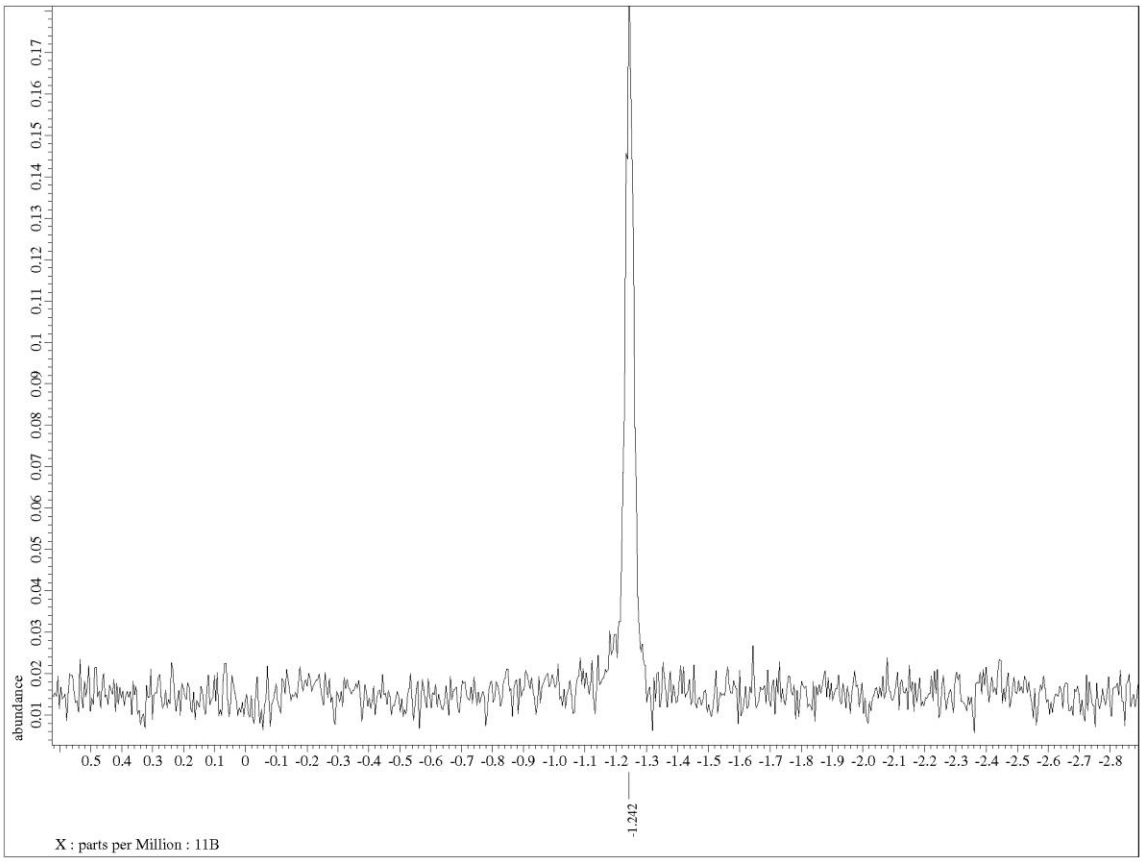


Figure S29. IR of $[CH_2(3,5\text{-}(CH_3)_2Pz)_2]Ag(CH_2{=}CHBF_3)$ **(6)**

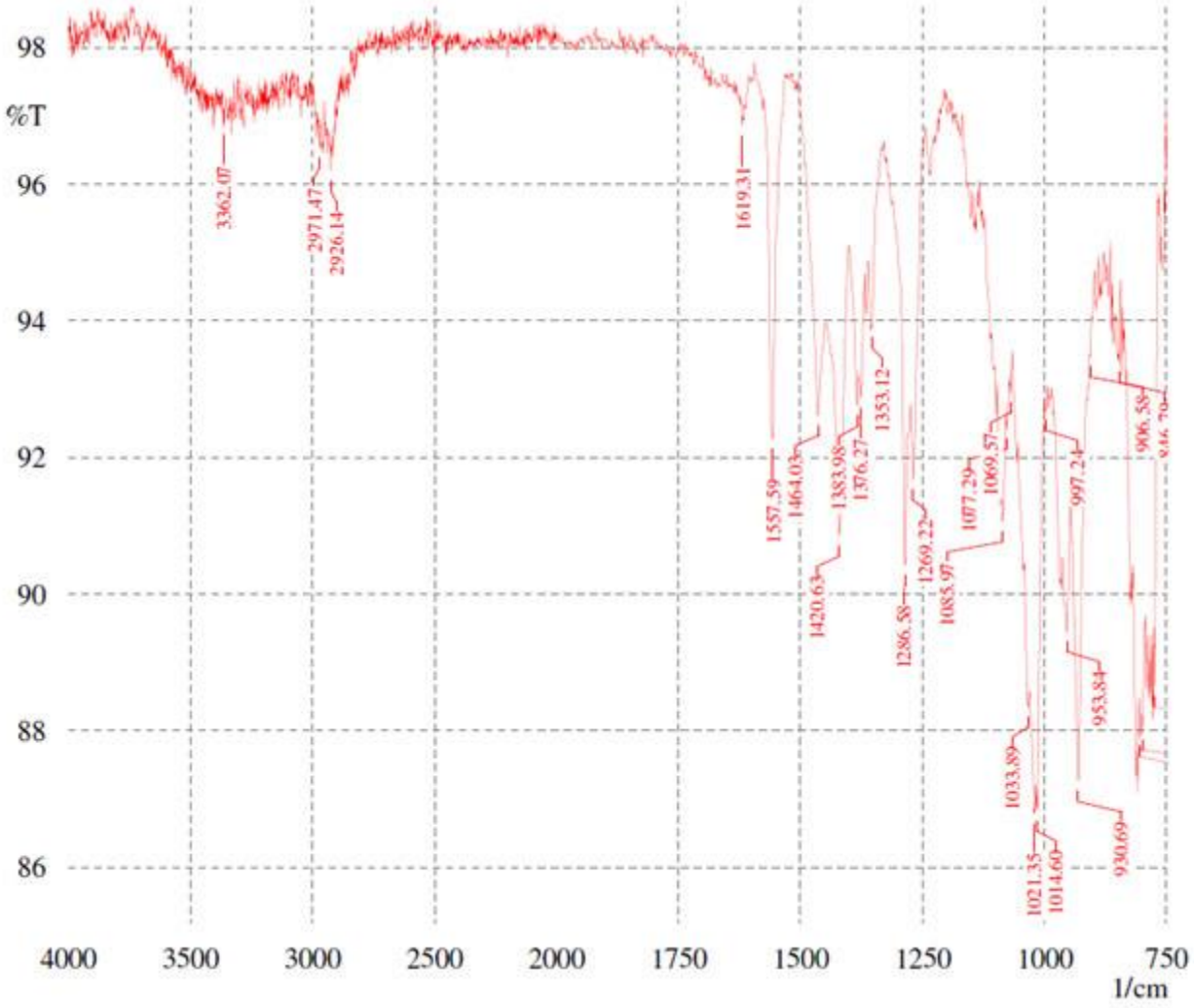


Figure S30. ^{19}F NMR of crude mixture of *cis/trans* potassium 2-(ethoxycarbonyl)cycloproyl trifluoroborate and unreacted $K(CH_2=CHBF_3)$

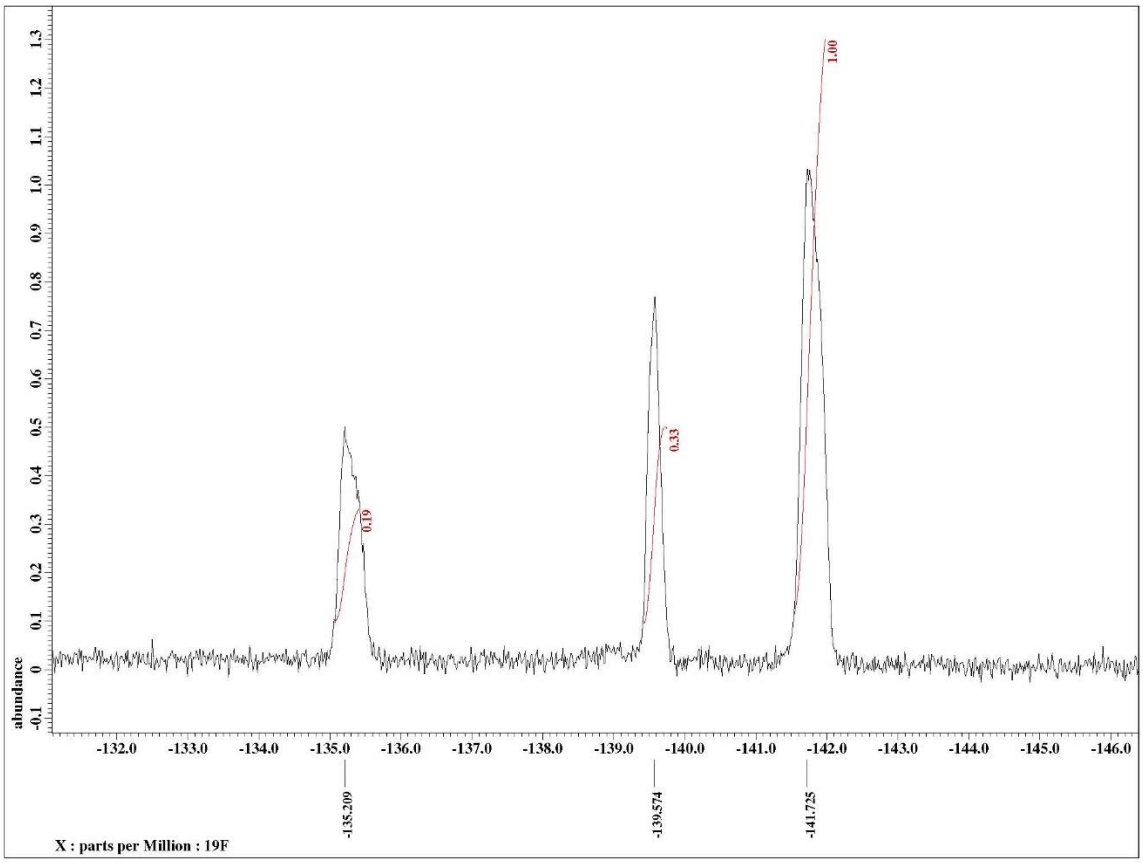
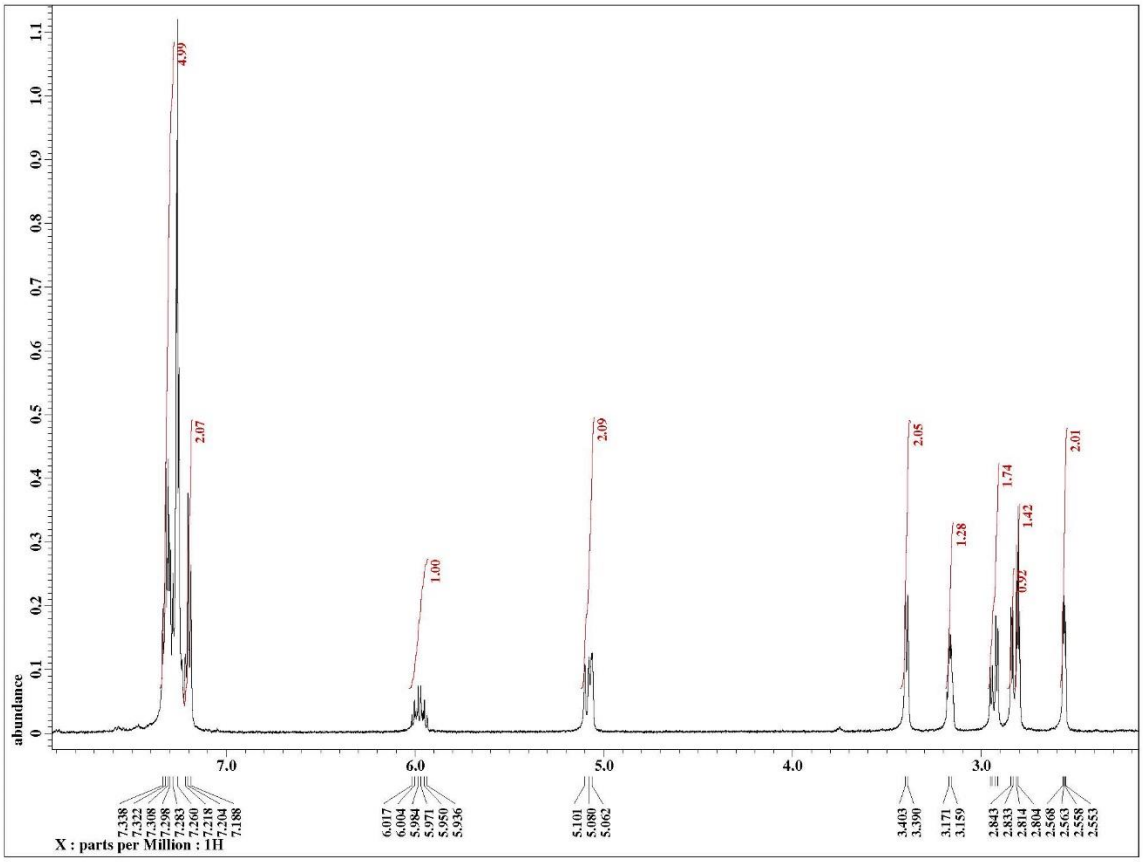


Figure S31. ^{1}H NMR of crude 1-phenylpent-4-en-2-ol



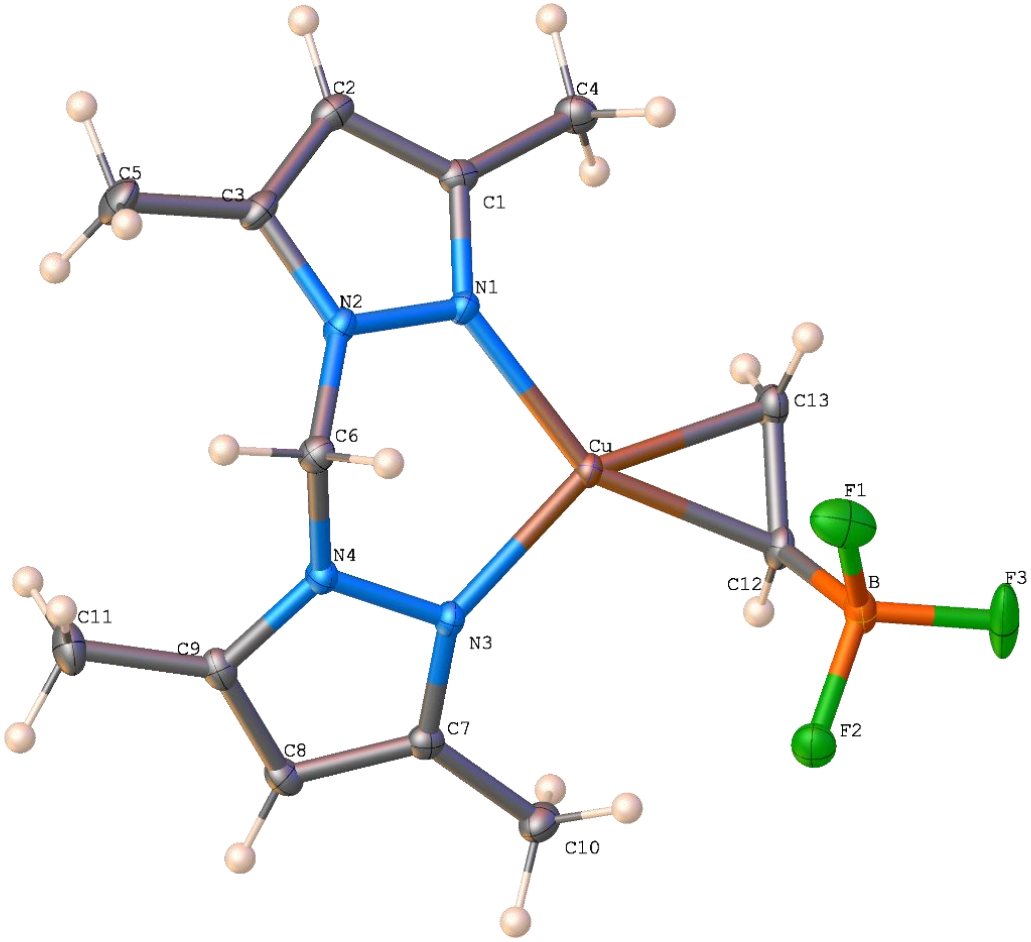


Table S2. Crystal data and structure refinement for $[CH_2(3,5\text{-}(CH_3)_2Pz)_2]Cu(CH_2{=}CHBF_3)$.

Empirical formula	$C_{13}H_{19}BCuF_3N_4$
Formula weight	362.67
Temperature/K	100.0
Crystal system	monoclinic
Space group	C2/c
a/Å	22.2814(7)
b/Å	7.8139(3)

c/Å	20.3486(10)
α/°	90
β/°	122.0380(10)
γ/°	90
Volume/Å^3	3003.2(2)
Z	8
ρ_{calc}g/cm^3	1.604
μ/mm^{-1}	1.487
F(000)	1488.0
Crystal size/mm^3	0.2 × 0.19 × 0.09
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.544 to 66.278
Index ranges	-34 ≤ h ≤ 34, -12 ≤ k ≤ 12, -31 ≤ l ≤ 31
Reflections collected	23153
Independent reflections	5707 [R_{int} = 0.0387, R_{sigma} = 0.0355]
Data/restraints/parameters	5707/0/215
Goodness-of-fit on F^2	1.040
Final R indexes [I>=2σ (I)]	R_1 = 0.0381, wR_2 = 0.0844
Final R indexes [all data]	R_1 = 0.0524, wR_2 = 0.0892
Largest diff. peak/hole / e Å^{-3}	1.50/-0.96

Table S3. Bond Lengths for $[CH_2(3,5\text{-}(CH_3)_2Pz)_2]Cu(CH_2{=}CHBF_3)$.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cu	N1	1.9941(14)	N4	C6	1.442(2)
Cu	N3	1.9910(14)	N4	C9	1.357(2)
Cu	C12	2.0488(16)	C1	C2	1.400(2)
Cu	C13	2.0279(17)	C1	C4	1.490(2)
F1	B	1.419(2)	C2	C3	1.381(2)
F2	B	1.411(2)	C3	C5	1.489(2)
F3	B	1.406(2)	C7	C8	1.402(2)
N1	N2	1.3711(19)	C7	C10	1.489(2)
N1	C1	1.342(2)	C8	C9	1.378(2)
N2	C3	1.360(2)	C9	C11	1.489(2)
N2	C6	1.445(2)	C12	C13	1.371(3)
N3	N4	1.3750(19)	C12	B	1.620(3)
N3	C7	1.342(2)			

Table S4. Bond Angles for $[CH_2(3,5\text{-}(CH_3)_2Pz)_2]Cu(CH_2{=}CHBF_3)$.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1	Cu	C12	149.72(7)	N2	C3	C2	106.28(14)
N1	Cu	C13	110.74(7)	N2	C3	C5	122.98(16)
N3	Cu	N1	96.86(6)	C2	C3	C5	130.74(16)
N3	Cu	C12	113.43(7)	N4	C6	N2	111.99(13)
N3	Cu	C13	151.43(7)	N3	C7	C8	109.97(14)
C13	Cu	C12	39.31(7)	N3	C7	C10	122.00(15)
N2	N1	Cu	119.87(11)	C8	C7	C10	128.03(16)
C1	N1	Cu	133.40(11)	C9	C8	C7	106.90(15)
C1	N1	N2	105.56(13)	N4	C9	C8	106.03(14)
N1	N2	C6	119.66(13)	N4	C9	C11	123.77(16)
C3	N2	N1	111.46(14)	C8	C9	C11	130.16(16)
C3	N2	C6	128.59(14)	C13	C12	Cu	69.52(10)
N4	N3	Cu	117.14(10)	C13	C12	B	N
C7	N3	Cu	129.77(11)	B	C12	Cu	110.16(11)
C7	N3	N4	105.37(13)	C12	C13	Cu	71.17(10)
N3	N4	C6	118.26(13)	F1	B	C12	111.20(15)
C9	N4	N3	111.73(13)	F2	B	F1	107.27(15)
C9	N4	C6	129.48(14)	F2	B	C12	112.81(15)

Table S4. Bond Angles for $[CH_2(3,5\text{-}(CH_3)_2Pz)_2]Cu(CH_2{=}CHBF_3)$.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1	C1	C2	110.16(15)	F3	B	F1	108.54(16)
N1	C1	C4	122.14(15)	F3	B	F2	107.33(16)
C2	C1	C4	127.68(15)	F3	B	C12	109.53(15)
C3	C2	C1	106.54(15)				

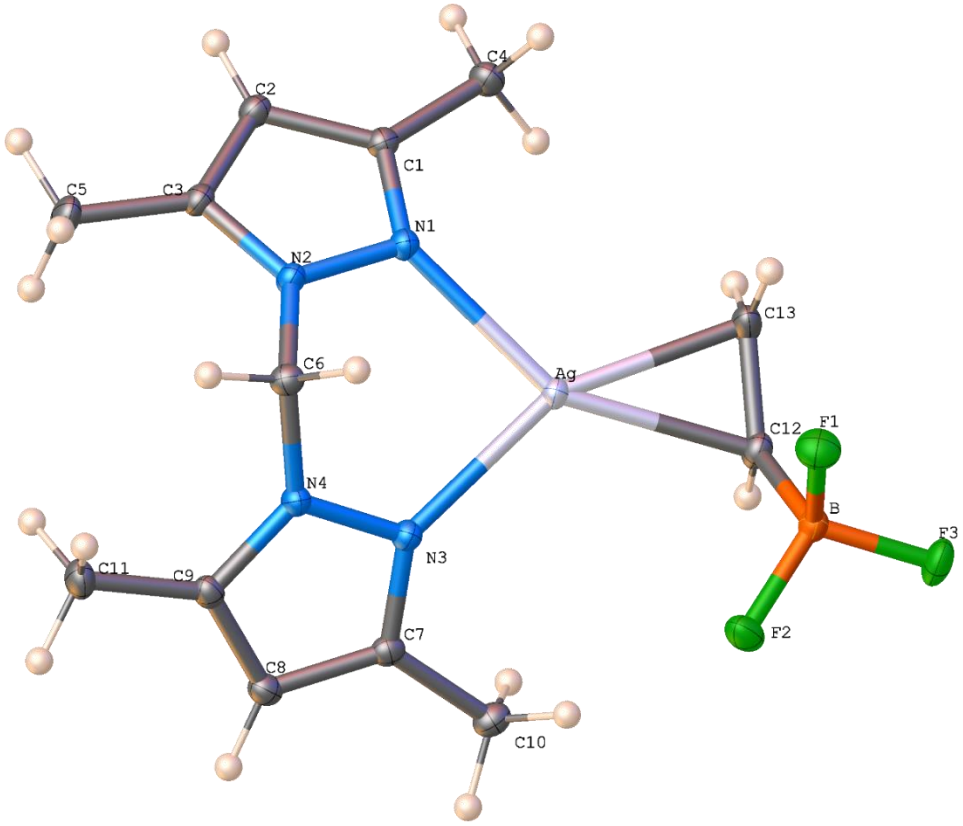


Table S5. Crystal data and structure refinement for $[CH_2(3,5\text{-}(CH_3)_2Pz)_2]Ag(CH_2{=}CHBF_3)$.

Empirical formula	$C_{13}H_{19}AgBF_3N_4$
Formula weight	407.00
Temperature/K	99.98
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	11.3966(6)
b/Å	12.1819(7)
c/Å	12.0151(7)
α/°	90
β/°	114.8850(10)
γ/°	90
Volume/Å^3	1513.21(15)
Z	4

ρ_{calc}g/cm^3	1.787
μ/mm^{-1}	1.364
F(000)	816.0
Crystal size/mm^3	0.47 × 0.36 × 0.14
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.014 to 76.166
Index ranges	$-19 \leq h \leq 19$, $-20 \leq k \leq 21$, $-20 \leq l \leq 20$
Reflections collected	30566
Independent reflections	7962 [R_{int} = 0.0262, R_{sigma} = 0.0253]
Data/restraints/parameters	7962/0/216
Goodness-of-fit on F^2	1.049
Final R indexes [I>=2σ (I)]	R_1 = 0.0243, wR_2 = 0.0589
Final R indexes [all data]	R_1 = 0.0294, wR_2 = 0.0612
Largest diff. peak/hole / e Å^{-3}	0.71/-1.12

Table S6. Bond Lengths for $[CH_2(3,5\text{-}(CH_3)_2Pz)_2]Ag(CH_2{=}CHBF_3)$.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ag	N1	2.2768(9)	N4	C6	1.4443(14)
Ag	N3	2.2454(9)	N4	C9	1.3597(13)
Ag	C12	2.3022(11)	C1	C2	1.4108(15)
Ag	C13	2.2562(11)	C1	C4	1.4886(15)
F1	B	1.4051(15)	C2	C3	1.3826(16)
F2	B	1.4078(14)	C3	C5	1.4910(16)
F3	B	1.4247(14)	C7	C8	1.4073(15)
N1	N2	1.3713(13)	C7	C10	1.4960(15)
N1	C1	1.3382(14)	C8	C9	1.3822(15)
N2	C3	1.3583(14)	C9	C11	1.4935(15)
N2	C6	1.4456(14)	C12	C13	1.3674(16)
N3	N4	1.3693(12)	C12	B	1.6300(17)
N3	C7	1.3386(13)			

Table S7. Bond Angles for $[CH_2(3,5\text{-}(CH_3)_2Pz)_2]Ag(CH_2{=}CHBF_3)$.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1	Ag	C12	150.45(4)	N2	C3	C2	106.19(9)
N3	Ag	N1	87.74(3)	N2	C3	C5	123.15(10)
N3	Ag	C12	121.61(4)	C2	C3	C5	130.64(10)
N3	Ag	C13	156.41(4)	N4	C6	N2	112.70(8)
C13	Ag	N1	115.61(4)	N3	C7	C8	110.18(9)
C13	Ag	C12	34.89(4)	N3	C7	C10	120.13(9)
N2	N1	Ag	117.94(6)	C8	C7	C10	129.67(10)
C1	N1	Ag	131.18(7)	C9	C8	C7	106.42(9)
C1	N1	N2	105.65(8)	N4	C9	C8	106.02(9)
N1	N2	C6	118.24(8)	N4	C9	C11	123.01(10)
C3	N2	N1	111.76(9)	C8	C9	C11	130.97(10)
C3	N2	C6	129.62(9)	C13	C12	Ag	70.71(6)
N4	N3	Ag	120.54(6)	C13	C12	B	124.95(11)
C7	N3	Ag	131.86(7)	B	C12	Ag	108.64(7)
C7	N3	N4	105.51(8)	C12	C13	Ag	74.39(7)
N3	N4	C6	118.92(8)	F1	B	F2	109.11(10)
C9	N4	N3	111.87(9)	F1	B	F3	107.50(9)

Table S7. Bond Angles for $[CH_2(3,5\text{-}(CH_3)_2Pz)_2]Ag(CH_2{=}CHBF_3)$.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C9	N4	C6	129.19(9)	F1	B	C12	111.85(9)
N1	C1	C2	110.04(9)	F2	B	F3	107.71(9)
N1	C1	C4	120.35(9)	F2	B	C12	111.97(9)
C2	C1	C4	129.60(10)	F3	B	C12	108.52(9)
C3	C2	C1	106.35(9)				

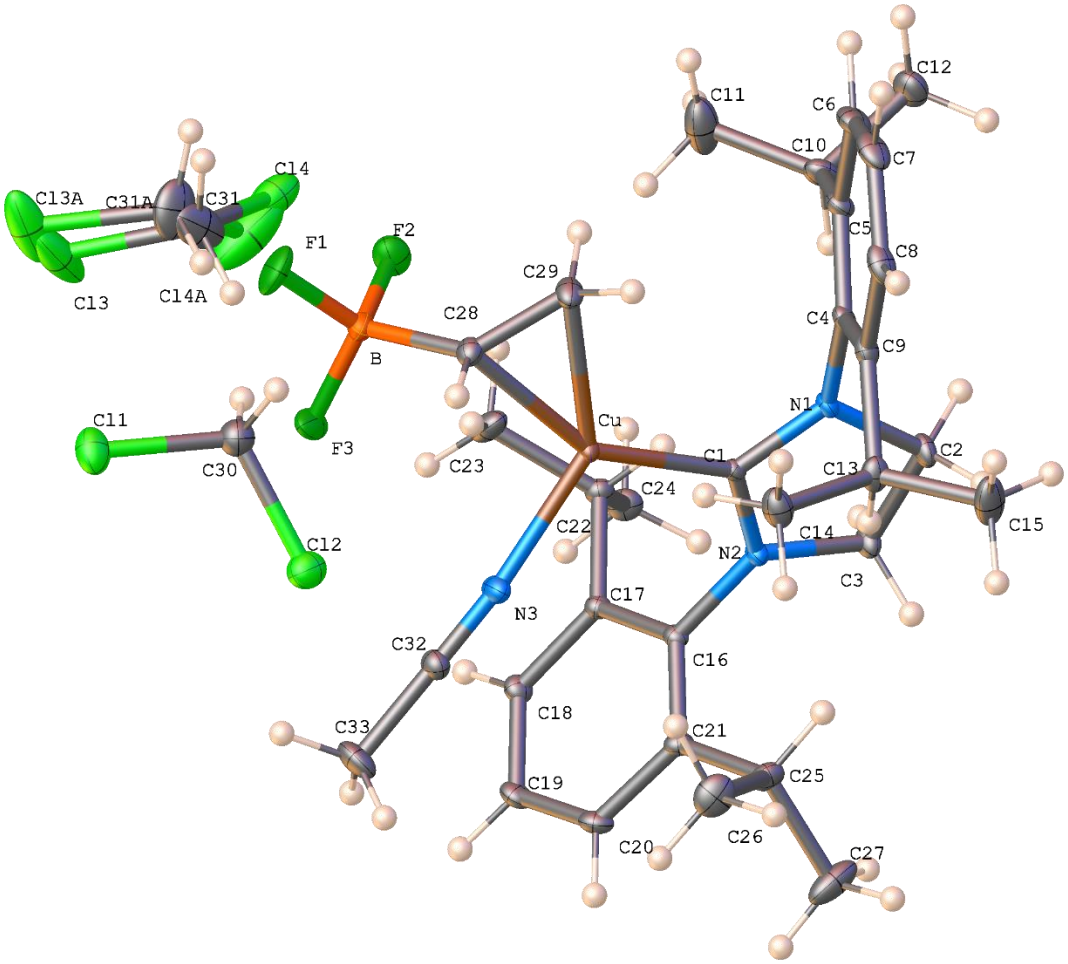


Table S8. Crystal data and structure refinement for (SIPr)Cu(MeCN)(CH_2=$CHBF_3$).

Empirical formula	$C_{33}H_{48}BCl_4CuF_3N_3$
Formula weight	759.89
Temperature/K	100.0
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	10.7461(4)
b/Å	22.3203(8)
c/Å	16.4600(6)
α/°	90
β/°	106.1390(10)
γ/°	90

Volume/$Å^3$	3792.4(2)
Z	4
$\rho_{calc}g/cm^3$	1.331
μ/mm^{-1}	0.899
F(000)	1584.0
Crystal size/mm^3	0.475 × 0.245 × 0.23
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.586 to 66.284
Index ranges	$-16 \leq h \leq 16$, $-34 \leq k \leq 34$, $-25 \leq l \leq 25$
Reflections collected	61121
Independent reflections	14453 [R_{int} = 0.0229, R_{sigma} = 0.0207]
Data/restraints/parameters	14453/30/454
Goodness-of-fit on F^2	1.026
Final R indexes [I>=2σ (I)]	R_1 = 0.0386, wR_2 = 0.1045
Final R indexes [all data]	R_1 = 0.0437, wR_2 = 0.1082
Largest diff. peak/hole / e $Å^{-3}$	1.07/-1.24

Table S9. Bond Lengths for (SIPr)Cu(MeCN)(CH_2=$CHBF_3$).

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cu	N3	1.9741(11)	C10	C12	1.524(2)
Cu	C1	1.9756(10)	C13	C14	1.5310(19)
Cu	C28	2.1061(12)	C13	C15	1.531(2)
Cu	C29	2.0936(13)	C16	C17	1.3998(15)
F1	B	1.4090(17)	C16	C21	1.4021(15)
F2	B	1.4075(18)	C17	C18	1.3972(16)
F3	B	1.4005(17)	C17	C22	1.5178(16)
N1	C1	1.3419(13)	C18	C19	1.3898(18)
N1	C2	1.4780(15)	C19	C20	1.3855(19)
N1	C4	1.4314(14)	C20	C21	1.3967(17)
N2	C1	1.3412(13)	C21	C25	1.5176(17)
N2	C3	1.4752(15)	C22	C23	1.5273(19)
N2	C16	1.4303(14)	C22	C24	1.5302(17)
N3	C32	1.1389(17)	C25	C26	1.526(2)
C2	C3	1.5288(17)	C25	C27	1.530(2)
C4	C5	1.3993(16)	C28	C29	1.3682(18)
C4	C9	1.4044(16)	C28	B	1.6187(19)
C5	C6	1.4002(18)	C32	C33	1.4537(19)
C5	C10	1.5175(19)	Cl1	C30	1.7636(17)
C6	C7	1.384(2)	Cl2	C30	1.7628(17)
C7	C8	1.385(2)	Cl3	C31	1.743(3)
C8	C9	1.3978(18)	Cl4	C31	1.745(4)
C9	C13	1.5157(19)	Cl3A	C31A	1.746(3)
C10	C11	1.528(3)	Cl4A	C31A	1.749(4)

Table S10. Bond Angles for (SIPr)Cu(MeCN)(CH_2=$CHBF_3$).

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N3	Cu	C1	112.78(4)	C9	C13	C15	111.58(12)
N3	Cu	C28	94.56(5)	C15	C13	C14	110.25(12)
N3	Cu	C29	131.81(5)	C17	C16	N2	118.89(10)
C1	Cu	C28	152.66(5)	C17	C16	C21	122.78(10)
C1	Cu	C29	114.99(5)	C21	C16	N2	118.33(10)
C29	Cu	C28	38.03(5)	C16	C17	C22	122.03(10)
C1	N1	C2	113.17(9)	C18	C17	C16	117.48(10)

Table S10. Bond Angles for (SIPr)Cu(MeCN)(CH_2=$CHBF_3$).

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C1	N1	C4	124.27(9)	C18	C17	C22	120.49(10)
C4	N1	C2	120.55(9)	C19	C18	C17	121.00(11)
C1	N2	C3	113.87(9)	C20	C19	C18	120.12(11)
C1	N2	C16	124.21(9)	C19	C20	C21	121.11(11)
C16	N2	C3	121.24(9)	C16	C21	C25	122.29(10)
C32	N3	Cu	174.50(12)	C20	C21	C16	117.43(11)
N1	C1	Cu	127.53(8)	C20	C21	C25	120.28(11)
N2	C1	Cu	125.26(8)	C17	C22	C23	112.04(10)
N2	C1	N1	107.21(9)	C17	C22	C24	110.30(10)
N1	C2	C3	102.12(9)	C23	C22	C24	110.79(11)
N2	C3	C2	101.40(9)	C21	C25	C26	111.95(12)
C5	C4	N1	118.53(10)	C21	C25	C27	110.97(11)
C5	C4	C9	122.63(11)	C26	C25	C27	109.94(13)
C9	C4	N1	118.83(10)	C29	C28	Cu	70.49(7)
C4	C5	C6	117.73(12)	C29	C28	B	122.87(12)
C4	C5	C10	121.34(11)	B	C28	Cu	109.52(8)
C6	C5	C10	120.92(12)	C28	C29	Cu	71.48(7)
C7	C6	C5	120.59(13)	N3	C32	C33	179.30(16)
C6	C7	C8	120.65(12)	F1	B	C28	110.12(11)
C7	C8	C9	120.95(13)	F2	B	F1	107.73(12)
C4	C9	C13	122.11(11)	F2	B	C28	110.28(11)
C8	C9	C4	117.38(12)	F3	B	F1	107.02(12)
C8	C9	C13	120.51(12)	F3	B	F2	107.23(12)
C5	C10	C11	112.03(14)	F3	B	C28	114.20(11)
C5	C10	C12	111.41(12)	Cl2	C30	Cl1	112.73(9)
C12	C10	C11	110.64(13)	Cl3	C31	Cl4	110.6(3)
C9	C13	C14	111.68(12)	Cl3A	C31A	Cl4A	111.8(4)

Table S11. Selected distances of optimized $M(CH_2=CH_2)$ structures.

	C=C bond length			M-C distance		
	$Cu(CH_2=CH_2)$	$Ag(CH_2=CH_2)$	$Au(CH_2=CH_2)$	$Cu(CH_2=CH_2)$	$Ag(CH_2=CH_2)$	$Au(CH_2=CH_2)$
wb97xd/def2tzvp	1.361	1.356	1.388	2.118	2.365	2.200
m06-2x/def2tzvp	1.352	1.350	1.385	2.229	2.454	2.205
bp86/def2tzvp	1.386	1.378	1.416	2.061	2.295	2.157
b3lyp/def2tzvp	1.366	1.361	1.395	2.136	2.378	2.210
pbe0/def2tzvp	1.364	1.360	1.395	2.099	2.329	2.165
ccsd(t)/def2qzvpp	1.358	1.357	1.395	2.173	2.372	2.164

Table S12. Metal-ethylene bond dissociation energies of $M(CH_2=CH_2)$ (in unit of kcal/mol).

	$Cu(CH_2=CH_2)$	$Ag(CH_2=CH_2)$	$Au(CH_2=CH_2)$
E-int (experiment)[2-4]	44-50	33.7	>59
wb97xd/def2tzvp	-46.75	-36.11	-60.30
m06-2x/def2tzvp	-43.05	-33.77	-54.30
bp86/def2tzvp	-58.26	-45.67	-76.87
b3lyp/def2tzvp	-48.55	-39.28	-64.93
pbe0/def2tzvp	-48.88	-39.40	-67.59
ccsd(t)/def2qzvpp	-41.41	-33.39	-63.00

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