Supporting Information

Direct *C*-Metallation of *N*-Substituted Triazoles Promoted by Mercury Acetate. An Alternative Route to *N*-Heterocyclic Carbene Complexes

Nai-Chieh Lin, Herbert J. H.Syu, Abbas Raja Naziruddin, Fu-Chen Liu*, Ivan J. B. Lin*

Department of Chemistry, National Dong Hwa University, Hualien 974, Taiwan, ROC

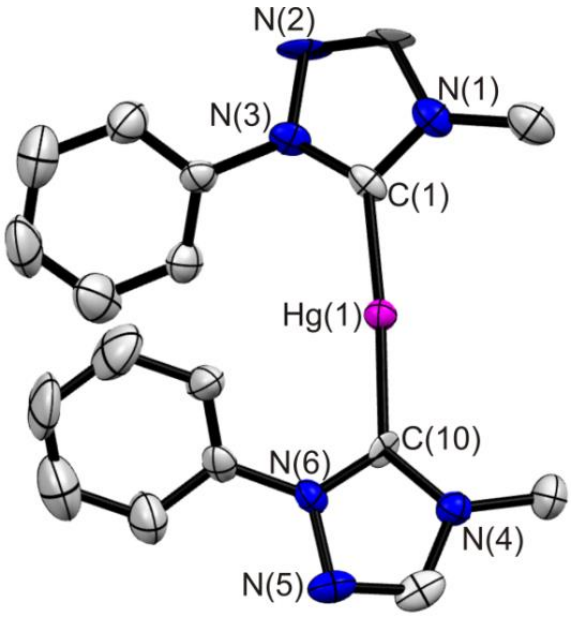


Figure S1: ORTEP of **3a**, depicted with 50% polarizability ellipsoids with hydrogen atoms and counter ions omitted for clarity.

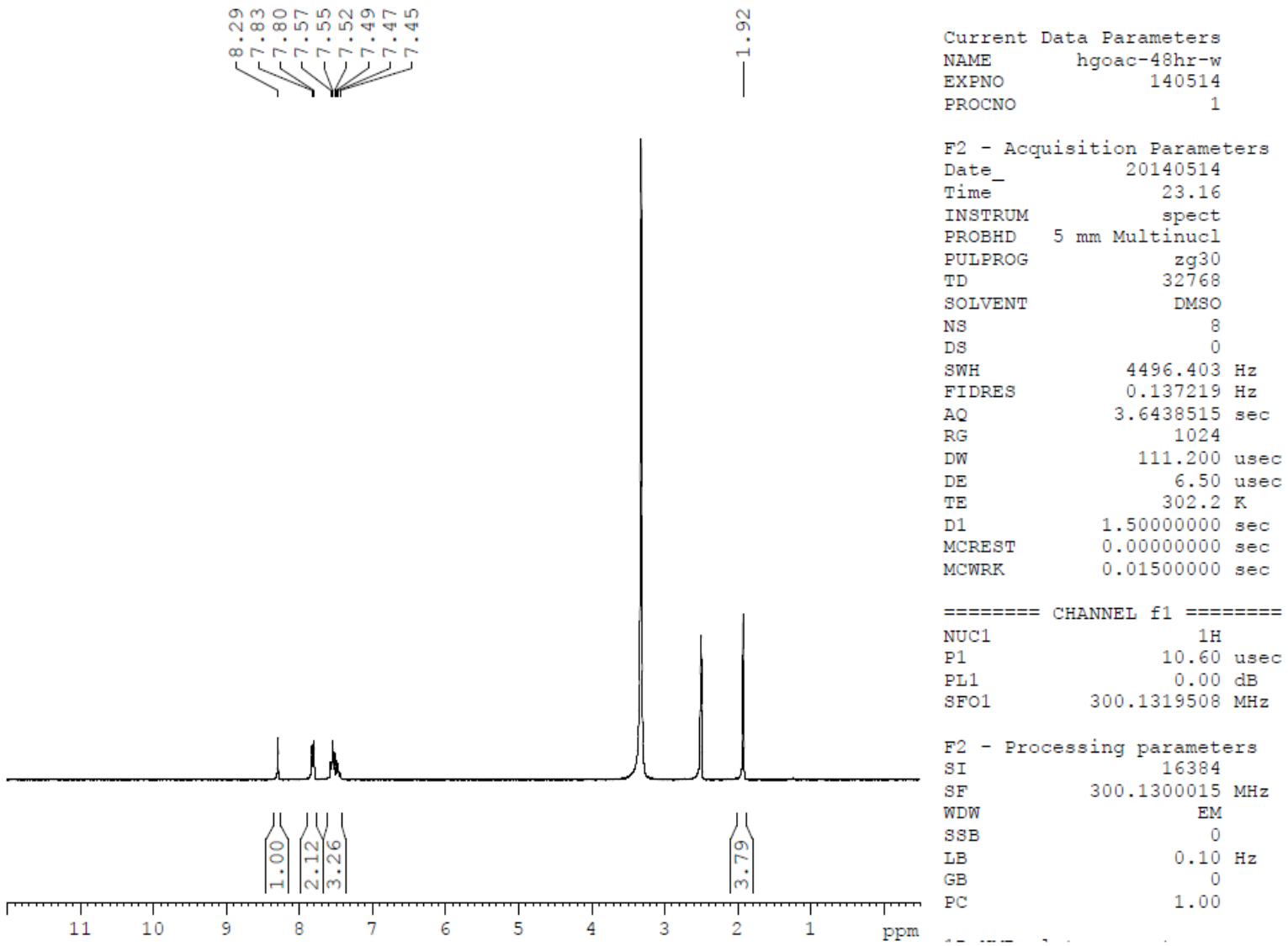
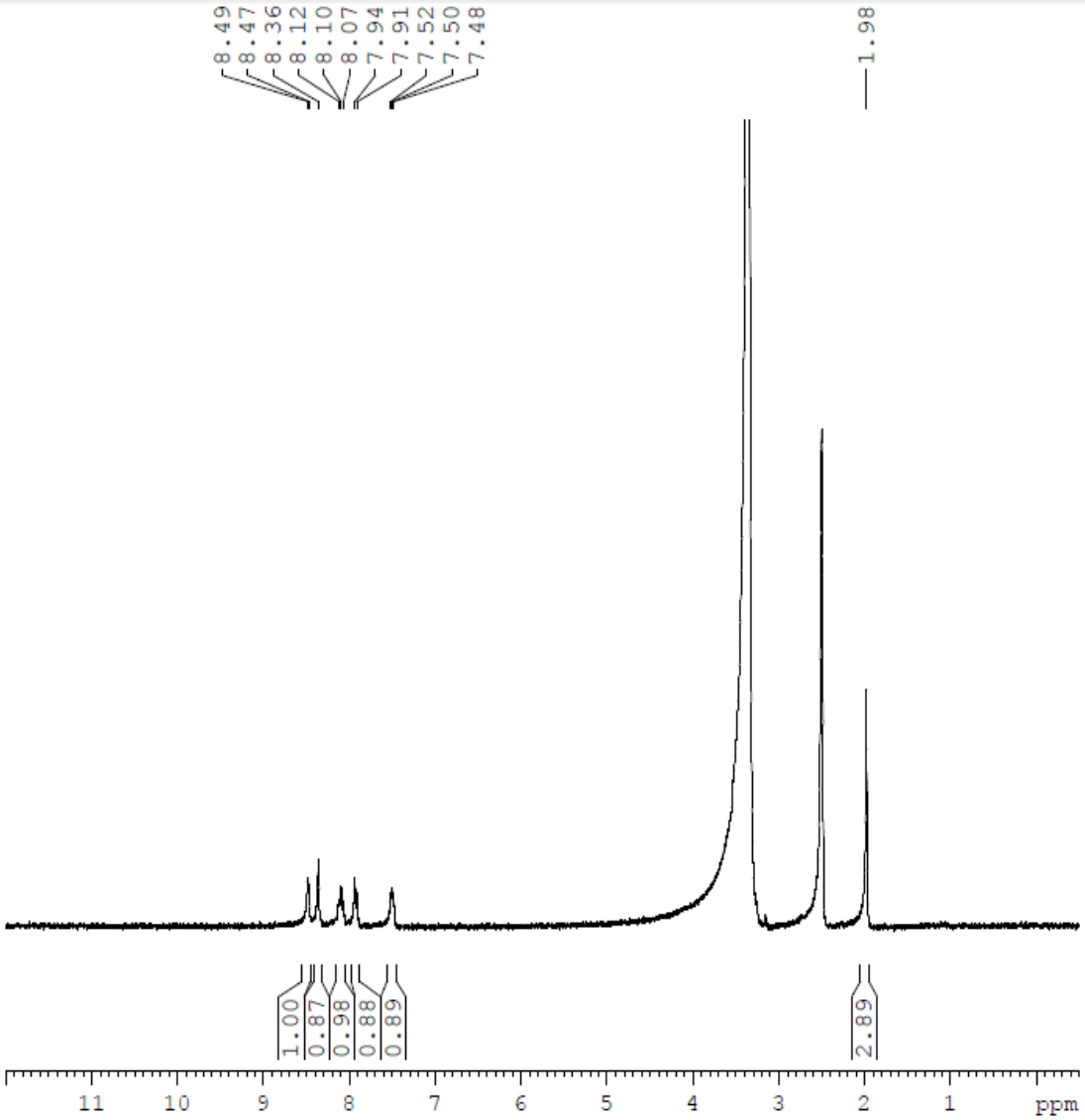


Figure S2: ^{1}H-NMR of **[Hg$_2$(Ph-Taz)$_2$(OAc)$_2$]$_\infty$ (1a)** in DMSO-d$_6$.




```
Current Data Parameters
NAME      hg-tripy-oac-s
EXPNO             140306
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140306
Time              12.18
INSTRUM             spect
PROBHD   5 mm Multinucl
PULPROG             zg30
TD                 32768
SOLVENT             DMSO
NS                    16
DS                     0
SWH             4496.403 Hz
FIDRES          0.137219 Hz
AQ             3.6438515 sec
RG                 645.1
DW              111.200 usec
DE                6.50 usec
TE                297.2 K
D1           1.50000000 sec
MCREST    0 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                 10.60 usec
PL1       0 dB
SFO1         300.1319508 MHz

F2 - Processing parameters
SI                 16384
SF           300.1300007 MHz
WDW                   EM
SSB       0
LB                 0.10 Hz
GB        0
PC                 1.00
```

Figure S3: ^{1}H-NMR of **[Hg$_2$(Py-Taz)$_2$(OAc)$_2$]$_\infty$ (1b)** in DMSO-d$_6$.

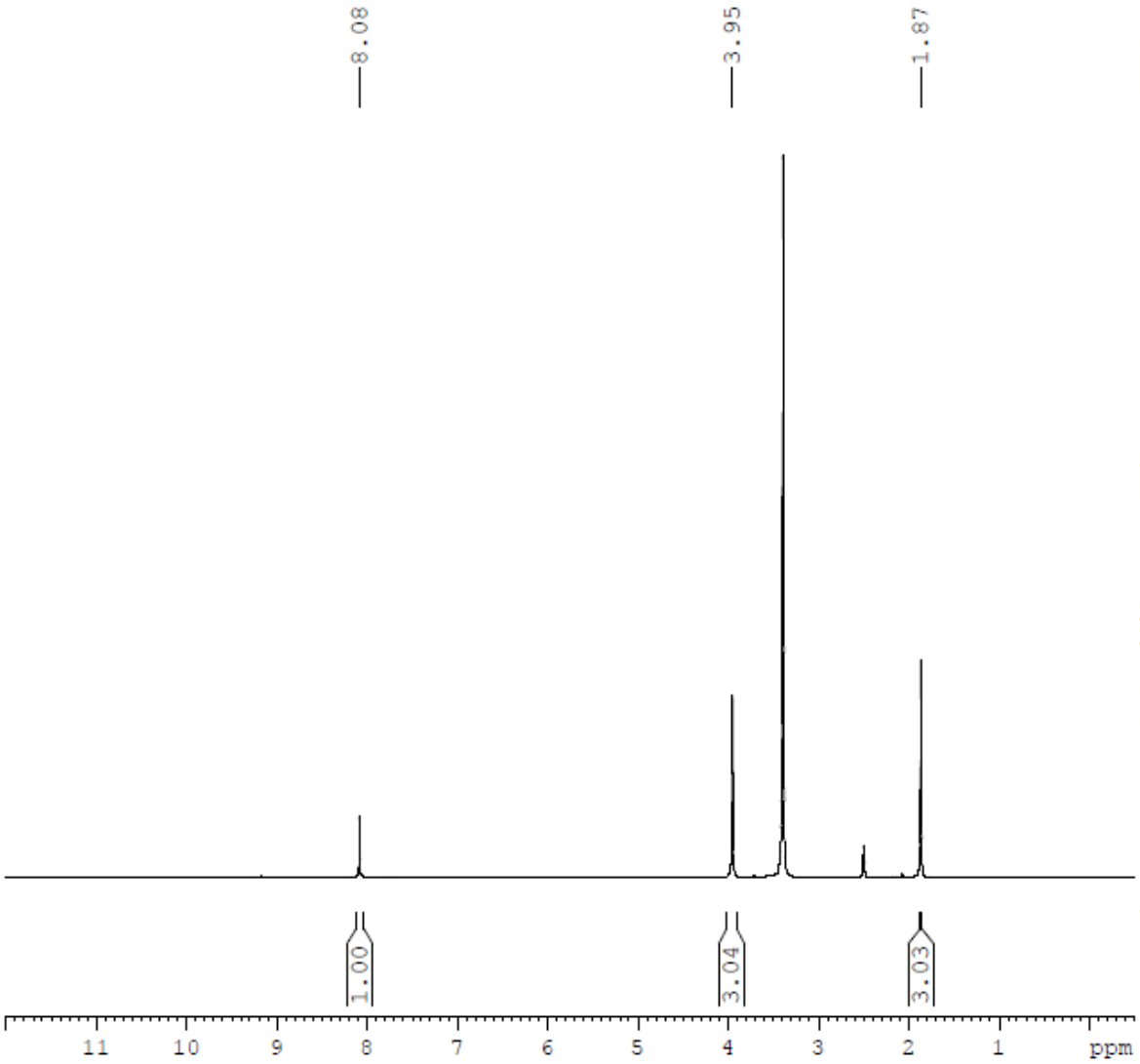


Figure S4: ^{1}H-NMR of [**Hg_2(Me-Taz)$_2$(OAc)$_2$]$_\infty$ (1c)** in DMSO-d_6.

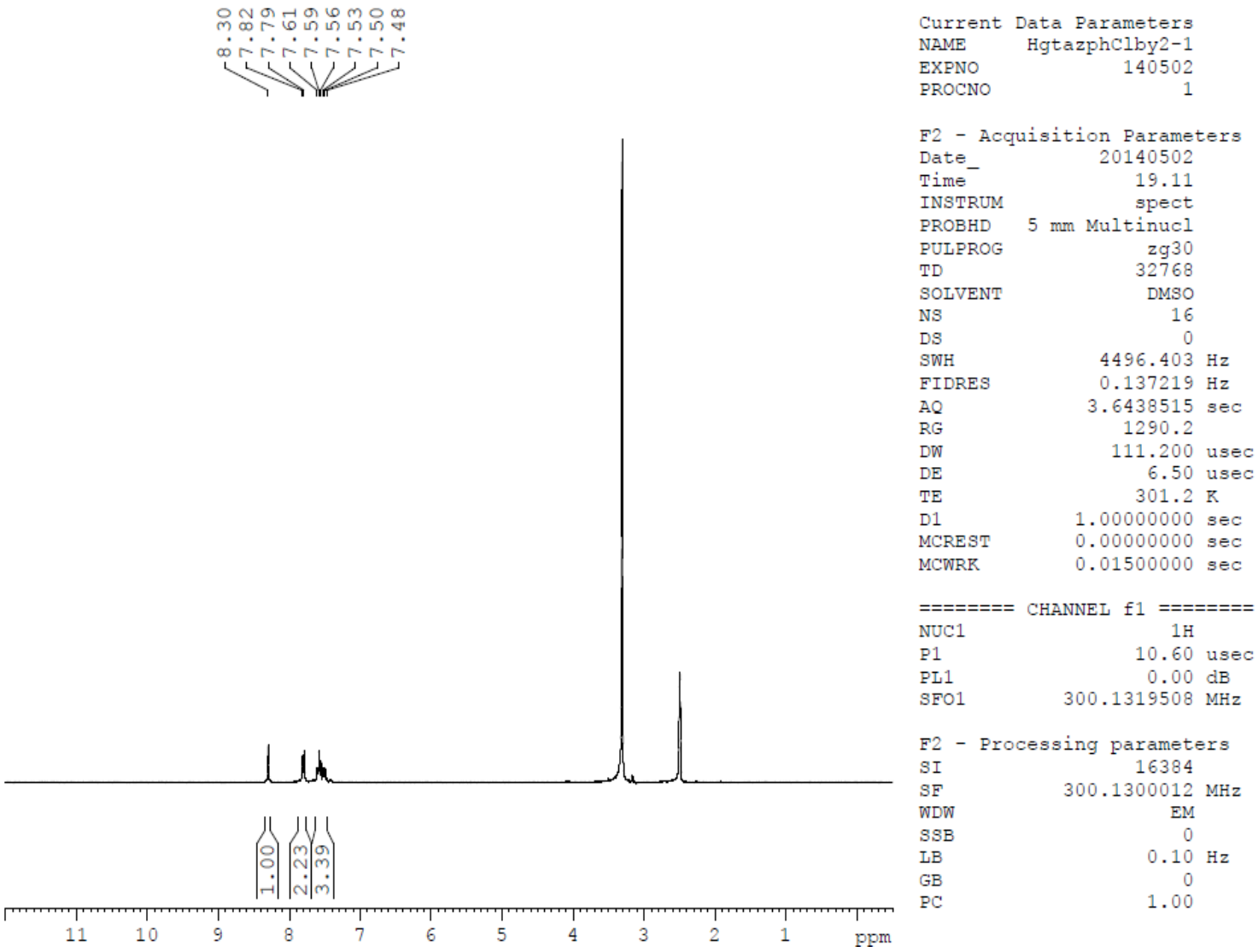
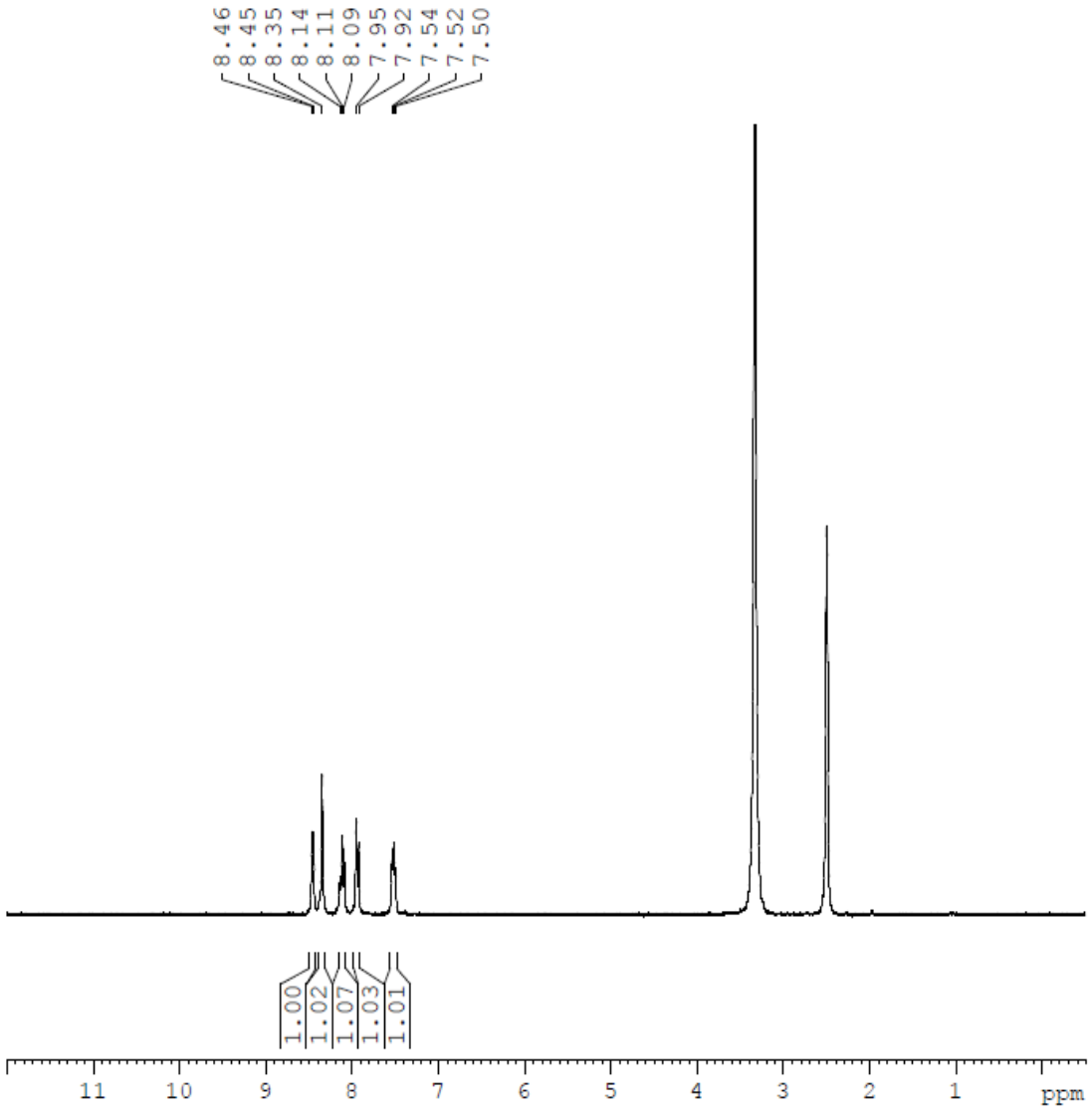


Figure S5: ^{1}H-NMR of [**Hg$_2$(Ph-Taz)$_2$(Cl)$_2$]$_\infty$ (2a**) in DMSO-d$_6$.




```
Current Data Parameters
NAME          hgtazprcl
EXPNO            140419
PROCNO                1

F2 - Acquisition Parameters
Date_          20140419
Time              13.52
INSTRUM           spect
PROBHD   5 mm Multinucl
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            4496.403 Hz
FIDRES         0.137219 Hz
AQ             3.6438515 sec
RG                724.1
DW              111.200 usec
DE                6.50 usec
TE                299.2 K
D1            1.50000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                10.60 usec
PL1                0.00 dB
SFO1        300.1319508 MHz

F2 - Processing parameters
SI                16384
SF          300.1300015 MHz
WDW                  EM
SSB                   0
LB                 0.10 Hz
GB                    0
PC                 1.00
```

Figure S6: ^{1}H-NMR of [**Hg$_2$(Py-Taz)$_2$(Cl)$_2$]$_\infty$** (**2b**) in DMSO-d$_6$.

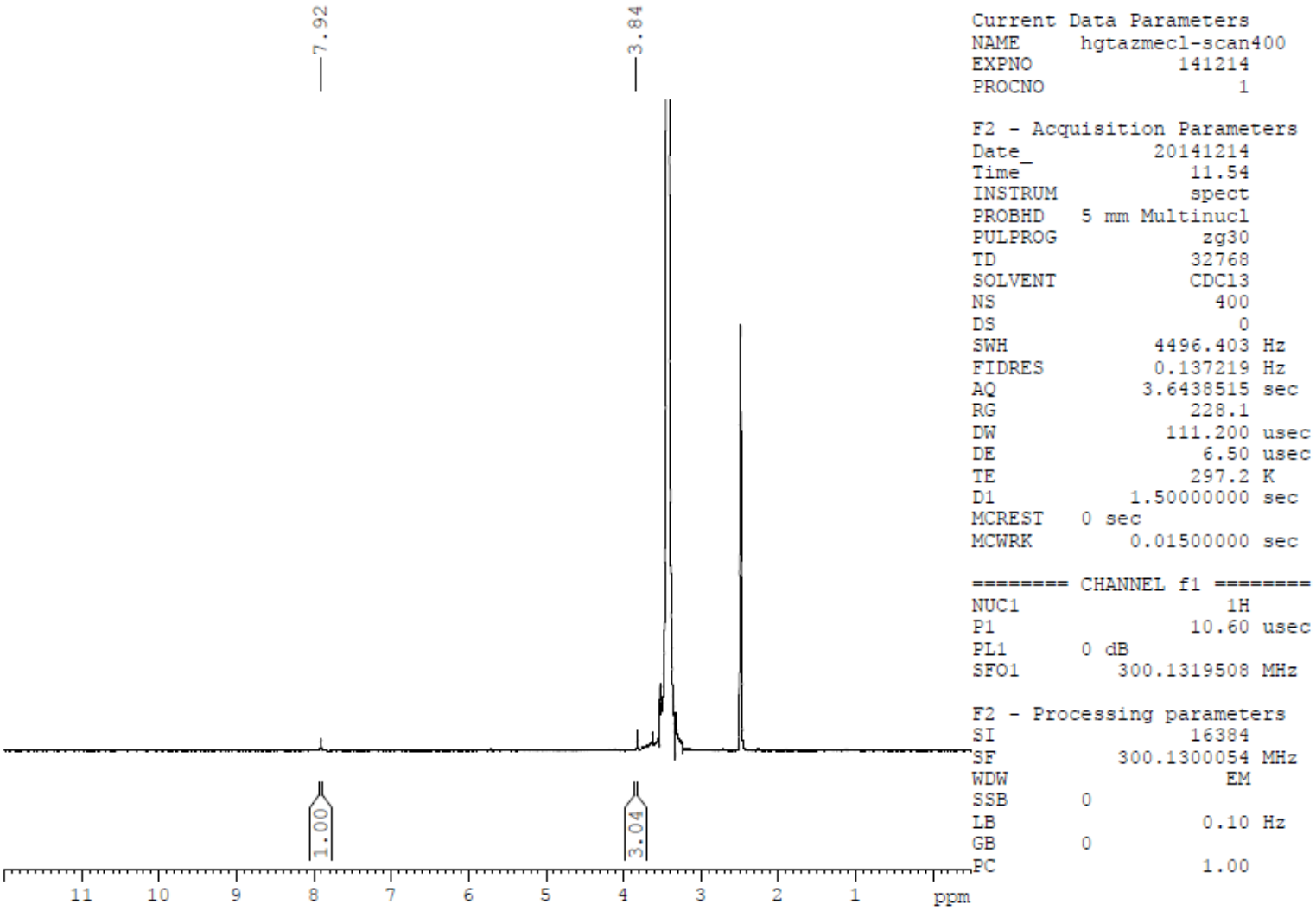


Figure S7: ^{1}H-NMR of [**Hg$_2$(Me-Taz)$_2$(Cl)$_2$]$_\infty$ (2c)** in DMSO-d$_6$.

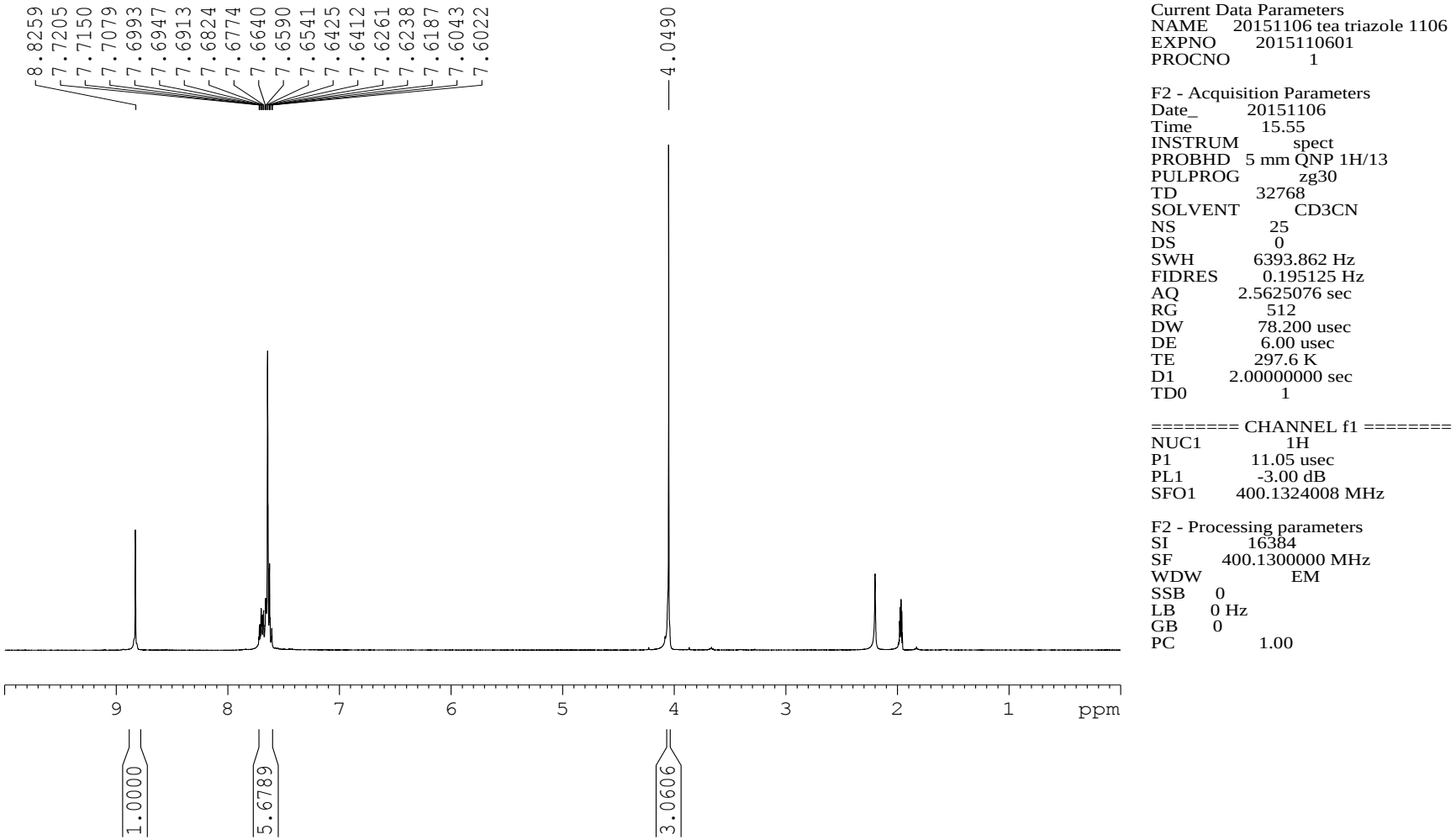


Figure S8: ^{1}H-NMR of **[(Ph-Taz-Me)$_2$Hg][BF$_4$]$_2$ (3a)** in CD_3CN.

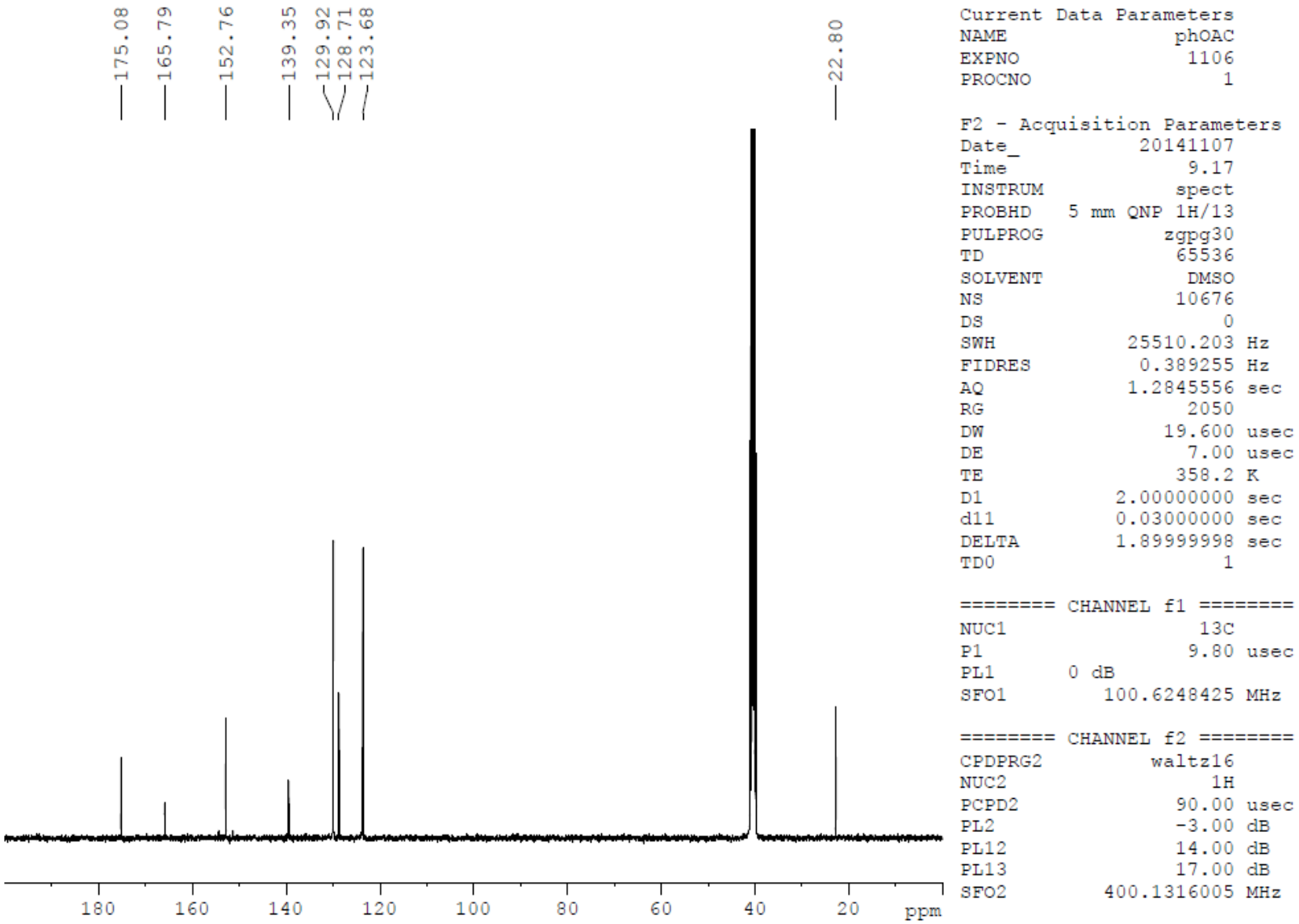


Figure S9: ^{13}C-NMR of [**Hg_2(Ph-Taz)$_2$(OAc)$_2$]$_\infty$ (1a)** in DMSO-d_6.

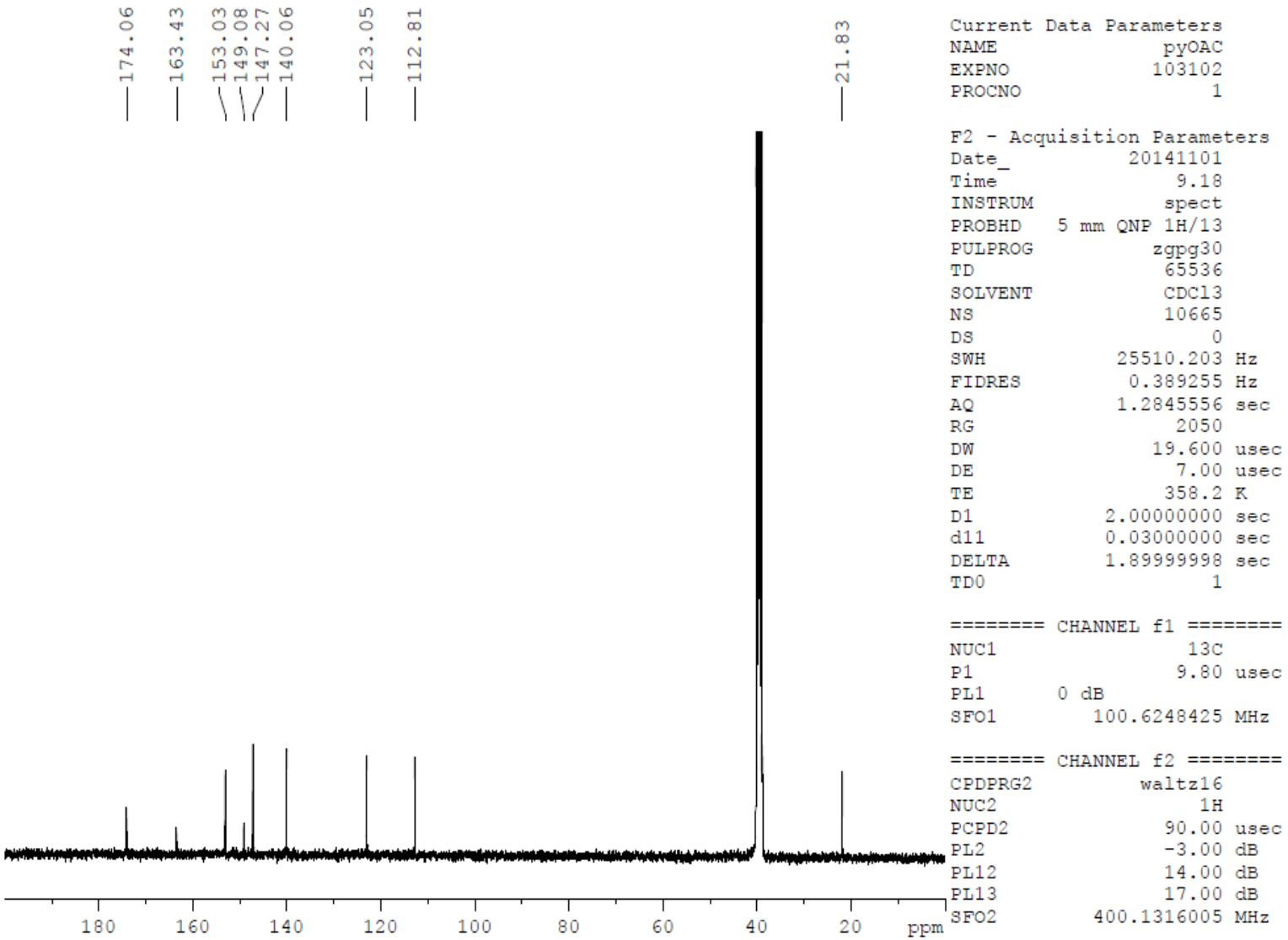


Figure S10: ^{13}C-NMR of [**Hg_2(Py-Taz)$_2$(OAc)$_2$]$_\infty$ (1b)** in DMSO-d_6.

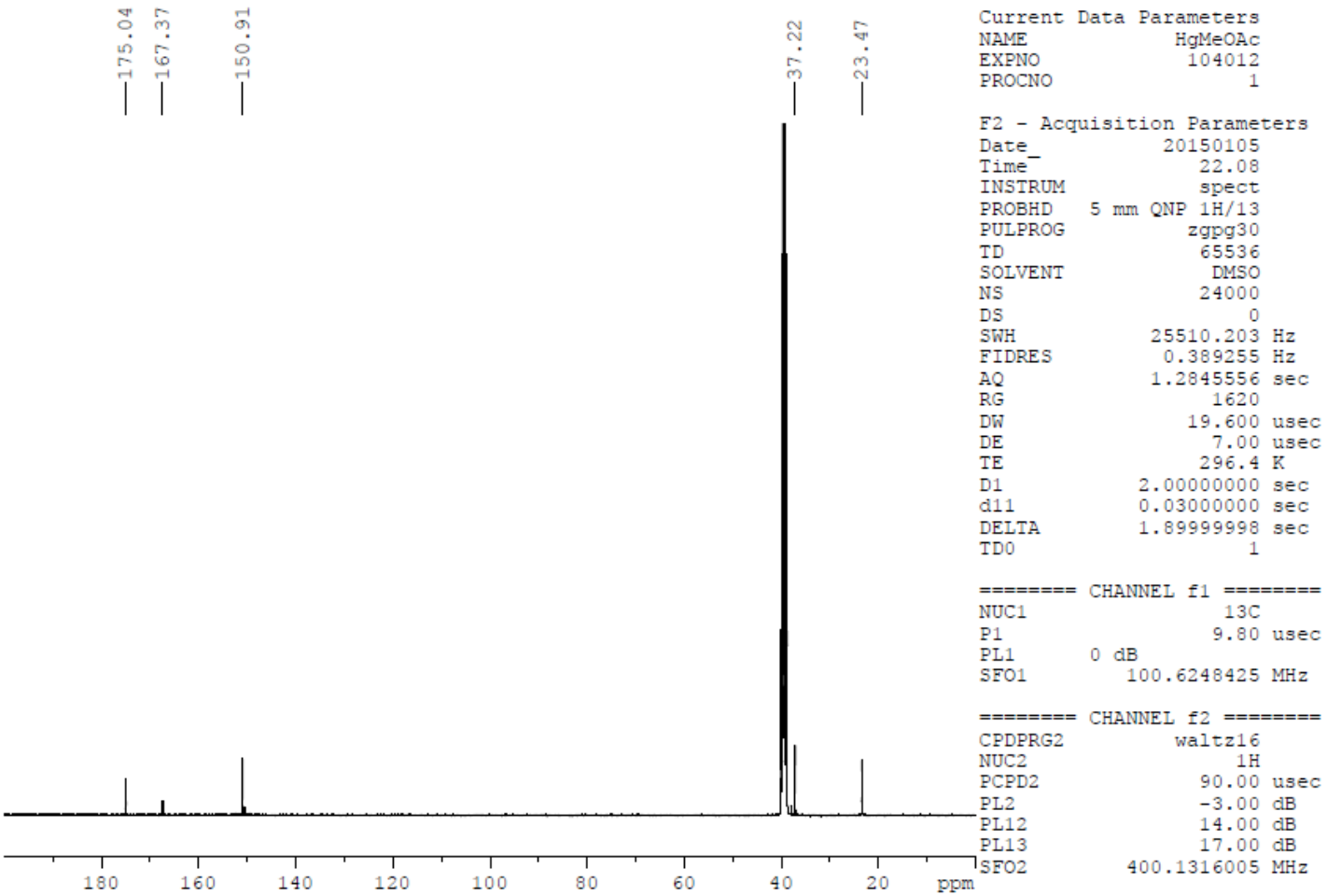


Figure S11: ^{13}C-NMR of [**Hg$_2$(Me-Taz)$_2$(OAc)$_2$]$_\infty$ (1c)** in DMSO-d$_6$.

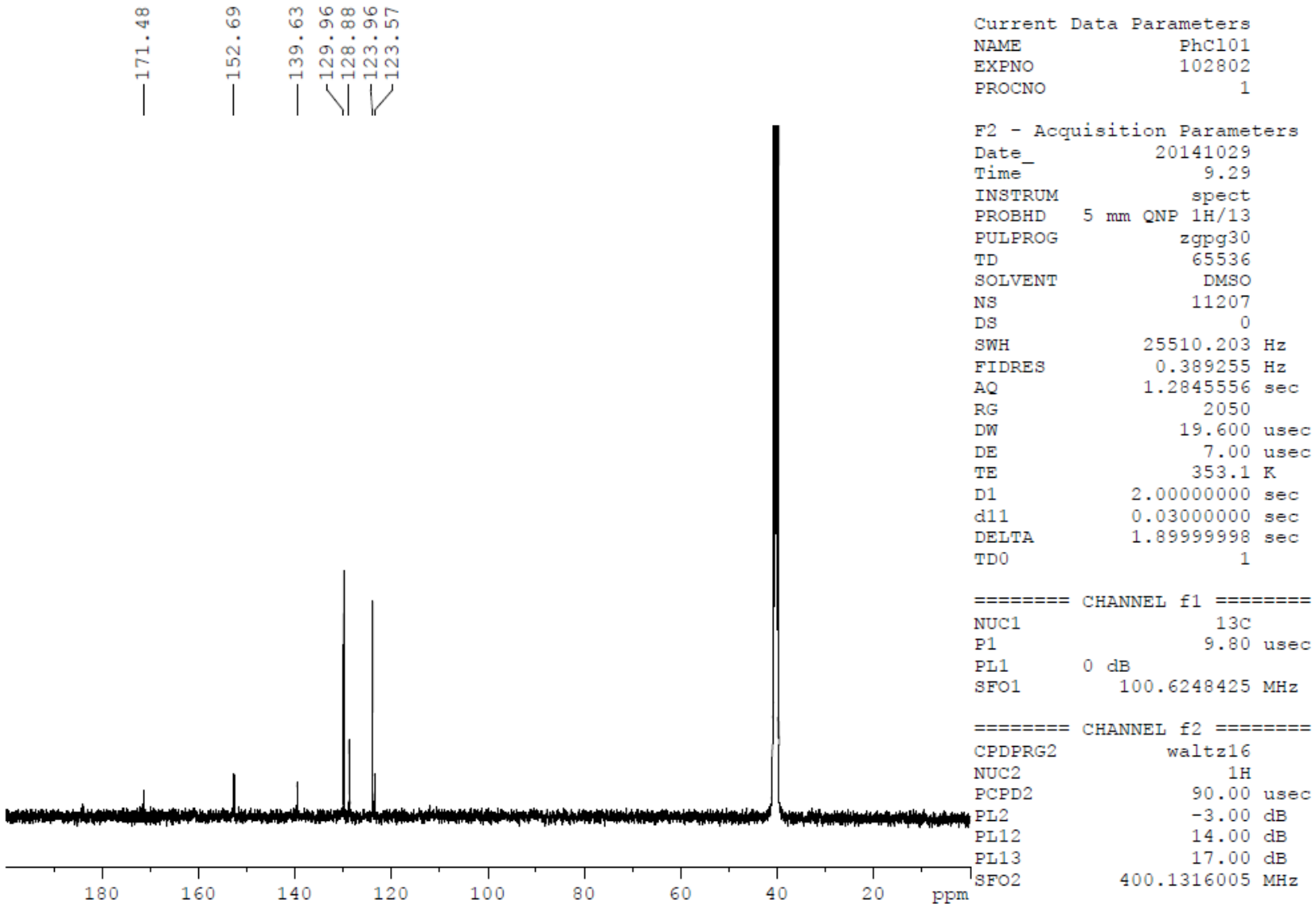


Figure S12: ^{13}C-NMR of [**Hg_2(Ph-Taz)$_2$($Cl)_2]_\infty$ (2a)** in DMSO-d_6.

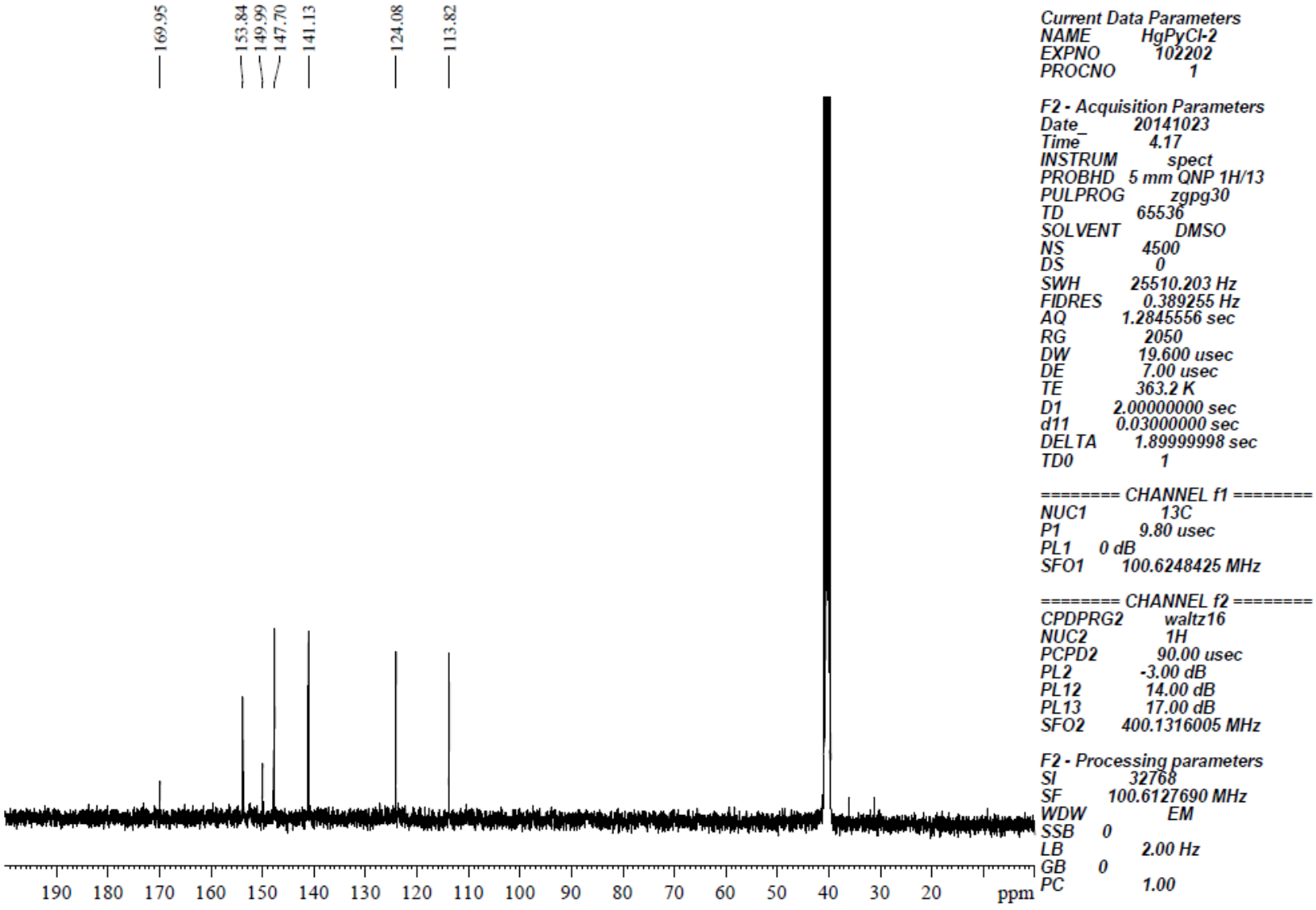


Figure S13: ^{13}C-NMR of [**Hg_2(Py-Taz)$_2$($Cl)_2$]$_\infty$ (2b)** in DMSO-d_6.

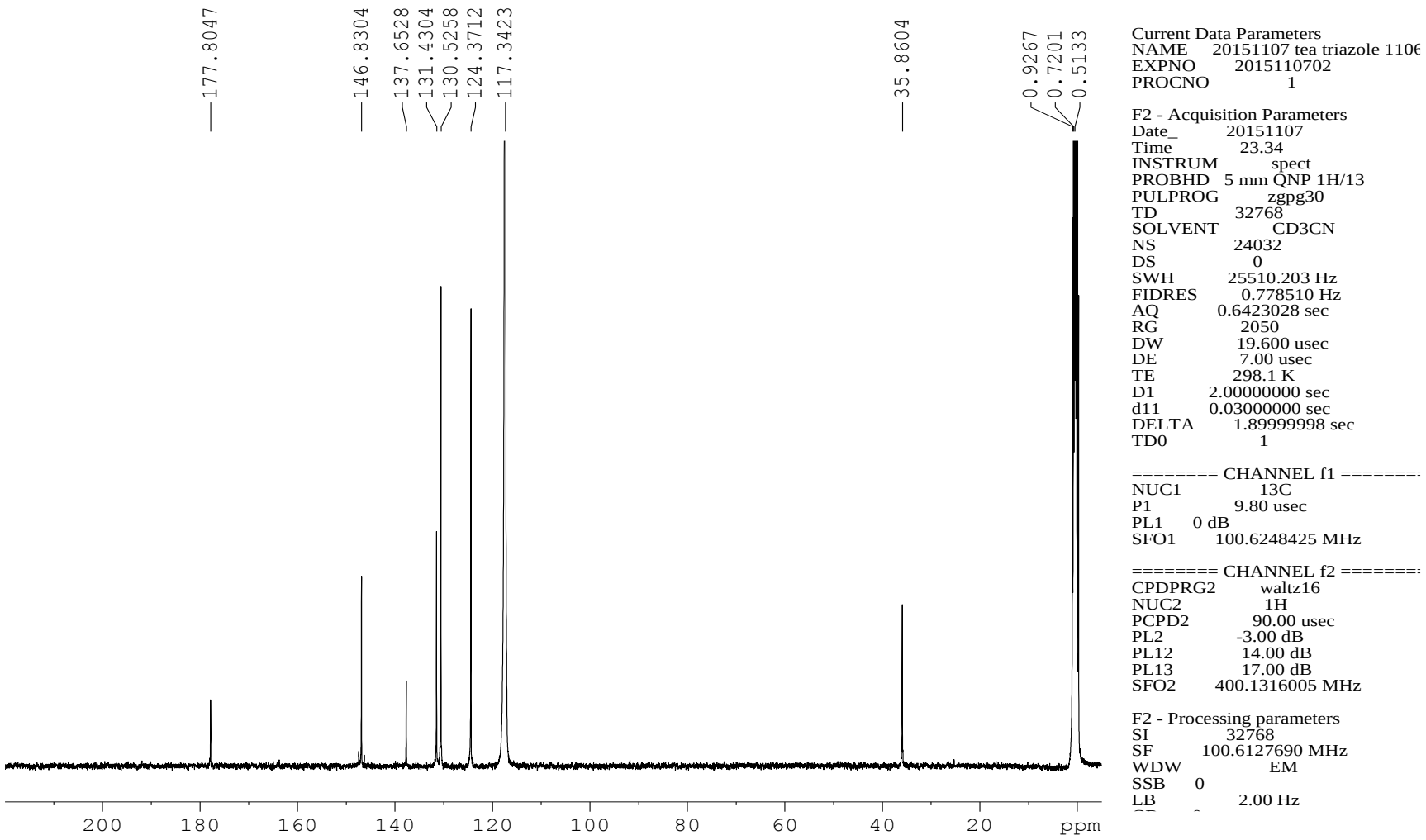


Figure S14: ^{13}C-NMR of **[(Ph-Taz-Me)$_2$Hg][BF$_4$]$_2$ (3a)** in CD_3CN.

Table S1. Crystal data and structure refinement for **1a**.

Empirical formula	$C_{10}H_9HgN_3O_2$	
Formula weight	403.79	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P(-)1	
Unit cell dimensions	a = 4.3353(9) Å	α = 106.28(3)°.
	b = 10.658(2) Å	β = 93.90(3)°.
	c = 12.488(3) Å	γ = 95.40(3)°.
Volume	548.7(2) $Å^3$	
Z	2	
Density (calculated)	2.444 Mg/m^3	
Absorption coefficient	14.012 mm^{-1}	
F(000)	372	
Crystal size	0.10 x 0.08 x 0.05 mm^3	
Theta range for data collection	1.707 to 26.468°.	
Index ranges	-5<=h<=5, -13<=k<=13, -15<=l<=15	
Reflections collected	5327	
Independent reflections	2271 [R(int) = 0.0301]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	multi-scan SADABS	
Max. and min. transmission	0.7454 and 0.4403	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2271 / 0 / 146	
Goodness-of-fit on F^2	0.983	
Final R indices [I>2sigma(I)]	R1 = 0.0273, wR2 = 0.0607	
R indices (all data)	R1 = 0.0369, wR2 = 0.0645	
Largest diff. peak and hole	1.297 and -1.053 e.$Å^{-3}$	

[a] $R_1 = \Sigma||F_o| - |F_c|| / \Sigma|F_o|$.

[b] $wR_2 = \{\Sigma w(F_o^2 - F_c^2)^2 / \Sigma w(F_o^2)^2\}^{1/2}$.

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **1a**.

Atom	x	y	z	U(eq)[a]
C(1)	3198(15)	3667(5)	3551(5)	42(14)
C(2)	4650(2)	1954(6)	3847(6)	62(2)
C(3)	1339(15)	2612(6)	1509(5)	44(14)
C(4)	-888(16)	1614(7)	937(5)	55(17)
C(5)	-2089(19)	1565(8)	-141(6)	70(2)
C(6)	-1029(19)	2519(8)	-612(6)	65(2)
C(7)	1235(19)	3516(7)	-20(6)	64(2)
C(8)	2451(17)	3568(7)	1040(5)	53(16)
C(9)	-1419(15)	7433(6)	3287(5)	46(14)
C(10)	-2223(18)	8794(7)	3323(7)	63(19)
Hg	2269(6)	5561(2)	3750(2)	45(10)
N(1)	2591(13)	2645(5)	2613(4)	45(12)
N(2)	3527(15)	1523(5)	2810(5)	58(15)
N(3)	4527(15)	3245(5)	4357(4)	57(15)
O(1)	1079(11)	7444(4)	3903(4)	55(11)
O(2)	-3045(11)	6439(4)	2731(4)	56(11)

[a] U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Table S3. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **1a**.

Atom	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C(1)	61(4)	27(3)	37(3)	3(3)	5(3)	8(2)
C(2)	101(6)	37(3)	50(4)	8(4)	-14(4)	19(3)
C(3)	60(4)	33(3)	34(3)	8(3)	1(3)	5(2)
C(4)	63(4)	51(4)	45(4)	-1(3)	-4(3)	9(3)
C(5)	66(5)	74(5)	56(4)	-6(4)	-11(4)	4(4)
C(6)	73(5)	79(5)	43(4)	14(4)	-7(3)	18(4)
C(7)	86(6)	60(4)	51(4)	7(4)	4(4)	27(4)
C(8)	61(4)	53(4)	46(4)	0(3)	3(3)	17(3)
C(9)	53(4)	38(3)	47(3)	5(3)	3(3)	14(3)
C(10)	61(5)	47(4)	81(5)	9(3)	-4(4)	23(4)
Hg	58(17)	30(13)	45(15)	4(10)	-4(10)	11(9)
N(1)	66(3)	32(2)	36(3)	4(2)	-3(2)	11(2)
N(2)	91(5)	31(3)	49(3)	11(3)	-8(3)	9(2)
N(3)	95(5)	31(3)	41(3)	3(3)	-12(3)	10(2)
O(1)	55(3)	35(2)	69(3)	7(2)	-6(2)	10(2)
O(2)	61(3)	44(3)	59(3)	2(2)	1(2)	12(2)

Table S4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å ^{2}x 10^3) for **1a**.

Atom	x	y	z	U(eq)
H(2)	5495	1407	4223	75
H(4)	-1599	971	1263	65
H(5)	-3605	888	-538	84
H(6)	-1832	2495	-1329	78
H(7)	1949	4162	-342	76
H(8)	3995	4236	1433	64
H(10A)	-2491	8865	2574	94
H(10B)	-568	9440	3749	94
H(10C)	-4118	8940	3670	94

Table S5. Bond lengths [Å] and angles [°] for **1a**.

Bond lengths			
C(1)-N(3)	1.330(8)	C(6)-C(7)	1.379(11)
C(1)-N(1)	1.348(7)	C(7)-C(8)	1.376(9)
C(1)-Hg	2.046(6)	C(9)-O(2)	1.217(8)
C(2)-N(2)	1.290(8)	C(9)-O(1)	1.282(8)
C(2)-N(3)	1.353(8)	C(9)-C(10)	1.513(9)
C(3)-C(4)	1.364(9)	Hg-O(1)	2.079(4)
C(3)-C(8)	1.375(9)	Hg-N(3)	2.583(5)
C(3)-N(1)	1.437(7)	N(1)-N(2)	1.377(7)
C(4)-C(5)	1.395(10)	N(3)-Hg	2.583(5)
C(5)-C(6)	1.370(11)		
Angles			
N(3)-C(1)-N(1)	108.5(5)	O(2)-C(9)-C(10)	122.2(6)
N(3)-C(1)-Hg	124.4(4)	O(1)-C(9)-C(10)	113.4(6)
N(1)-C(1)-Hg	127.1(4)	C(1)-Hg-O(1)	176.8(2)
N(2)-C(2)-N(3)	116.3(6)	C(1)-Hg-N(3)	100.8(2)
C(4)-C(3)-C(8)	121.3(6)	O(1)-Hg-N(3)	81.92(18)
C(4)-C(3)-N(1)	119.1(6)	C(1)-N(1)-N(2)	110.1(5)
C(8)-C(3)-N(1)	119.5(5)	C(1)-N(1)-C(3)	129.8(5)
C(3)-C(4)-C(5)	119.5(7)	N(2)-N(1)-C(3)	120.0(5)
C(6)-C(5)-C(4)	119.8(7)	C(2)-N(2)-N(1)	101.8(5)
C(5)-C(6)-C(7)	119.7(7)	C(1)-N(3)-C(2)	103.3(5)
C(8)-C(7)-C(6)	121.0(7)	C(1)-N(3)-Hg	133.1(4)
C(3)-C(8)-C(7)	118.7(7)	C(2)-N(3)-Hg	121.4(4)
O(2)-C(9)-O(1)	124.4(6)	C(9)-O(1)-Hg	112.3(4)

Symmetry transformations used to generate equivalent atoms:

Table S6. Crystal data and structure refinement for **2b**.

Empirical formula	$C_{14}H_{10}Cl_2Hg_2N_8$	
Formula weight	762.38	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 13.1710(18) Å	α = 90°.
	b = 4.5399(5) Å	β = 93.807(11) (3)°.
	c = 14.990(2) Å	γ = 90°.
Volume	894.3(2) $Å^3$	
Z	2	
Density (calculated)	2.831 Mg/m^3	
Absorption coefficient	17.461 mm^{-1}	
F(000)	688	
Crystal size	079 x 0.03 x 0.02 mm^3	
Theta range for data collection	3.100 to 24.995°.	
Index ranges	-15<=h<=15, -5<=k<=5, -16<=l<=17	
Reflections collected	5762	
Independent reflections	1571 [R(int) = 0.0308]	
Completeness to theta = 24.996°	99.4 %	
Absorption correction	multi-scan SADABS	
Max. and min. transmission	0.5574 and 0.2265	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1571/ 0 / 118	
Goodness-of-fit on F^2	1.369	
Final R indices [I>2sigma(I)]	R1 = 0.0571, wR2 = 0.1717	
R indices (all data)	R1 = 0.0633, wR2 = 0.1738	
Largest diff. peak and hole	2.752 and -2.013 e.$Å^{-3}$	

[a] $R_1 = \Sigma||F_o| - |F_c|| / \Sigma|F_o|$.

[b] $wR_2 = \{\Sigma w(F_o^2 - F_c^2)^2 / \Sigma w(F_o^2)^2\}^{1/2}$.

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å ^{2}x 10^3) for **2b**

Atom	x	y	z	U(eq)[a]
C(1)	3600(17)	390(6)	7930(16)	37(5)
C(2)	3627(19)	-180(6)	9351(15)	42(6)
C(3)	5004(18)	4040(6)	7941(15)	36(5)
C(4)	5660(2)	5540(5)	8468(15)	41(6)
C(5)	6350(2)	7300(7)	8054(19)	51(7)
C(6)	6300(2)	7470(7)	7110(2)	53(7)
C(7)	5570(2)	5840(6)	6655(19)	47(7)
N(1)	3148(15)	-1160(5)	8543(12)	42(5)
N(2)	4334(16)	1790(5)	9260(13)	43(5)
N(3)	4292(14)	2150(5)	8352(11)	34(5)
N(4)	4917(15)	4090(5)	7062(13)	38(5)
Cl	3333(6)	-580(2)	5046(4)	62(2)
Hg	3360(7)	275(2)	6560(6)	39(3)

[a] U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Table S8. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **2b.**

Atom	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C(1)	37(13)	37(14)	36(13)	-1(11)	-2(10)	6(11)
C(2)	50(15)	53(16)	23(11)	2(14)	-1(10)	4(12)
C(3)	34(12)	40(14)	33(12)	3(11)	-5(10)	10(11)
C(4)	72(18)	29(12)	23(11)	-9(13)	4(11)	-4(10)
C(5)	51(17)	48(16)	54(17)	-3(14)	-2(13)	-4(14)
C(6)	54(18)	50(17)	58(18)	10(15)	19(14)	8(15)
C(7)	45(15)	49(16)	47(15)	4(13)	10(12)	-1(13)
N(1)	40(11)	65(15)	20(9)	-12(11)	-8(8)	4(10)
N(2)	52(13)	52(13)	23(10)	-7(11)	-11(9)	3(10)
N(3)	38(11)	44(12)	17(9)	-1(9)	-12(8)	0(8)
N(4)	38(11)	39(12)	35(11)	2(10)	-6(9)	3(9)
Cl	77(5)	81(6)	29(3)	-5(5)	6(3)	-12(4)
Hg	45(6)	46(6)	26(5)	-3(5)	-3(3)	-3(4)

Table S9. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å ^{2}x 10^3) for **2b.**

Atom	x	y	z	U(eq)
H(2)	3456	-877	9905	51
H(4)	5666	5416	9087	50
H(5)	6838	8364	8394	61
H(6)	6745	8658	6819	64
H(7)	5530	5932	6033	56

Table S10. Bond lengths [Å] and angles [°] for **2b.**

	Bond lengths		
C(1)-N(1)	1.330(3)	C(3)-N(4)	1.310(3)
C(5)-C(6)	1.410(4)	N(1)-Hg	2.560(2)
C(1)-N(3)	1.340(3)	C(3)-C(4)	1.320(3)
C(1)-Hg	2.060(2)	N(2)-N(3)	1.370(2)
C(6)-C(7)	1.360(4)	C(3)-N(3)	1.440(3)
C(2)-N(2)	1.310(3)	Cl-Hg	2.301(6)
C(2)-N(1)	1.400(3)	C(4)-C(5)	1.380(4)
C(7)-N(4)	1.350(3)	Hg-N(1)	2.560(2)
N(4)-Hg	2.750(2)		
	Angles		
N(1)-C(1)-N(3)	108.0(2)	C(2)-N(2)-N(3)	101.7(19)
N(1)-C(1)-Hg	129.1(18)	C(3)-C(4)-C(5)	117.0(2)
N(3)-C(1)-Hg	122.9(17)	C(1)-N(3)-N(2)	112.0(2)
N(4)-C(7)-C(6)	123.0(3)	C(1)-N(3)-C(3)	126.5(19)
N(2)-C(2)-N(1)	114.0(2)	N(2)-N(3)-C(3)	120.8(19)
C(1)-N(1)-C(2)	104.0(2)	C(4)-C(5)-C(6)	120.0(3)
N(4)-C(3)-C(4)	127.0(2)	C(3)-N(4)-C(7)	117.0(2)
C(1)-N(1)-Hg	132.4(15)	C(1)-Hg-Cl	168.5(7)
N(4)-C(3)-N(3)	115.0(2)	C(1)-Hg-N(1)	96.4(8)
C(2)-N(1)-Hg	123.8(16)	C(7)-C(6)-C(5)	117.0(3)
C(4)-C(3)-N(3)	118.0(2)	Cl-Hg-N(1)	95.0(5)
N(4)-Hg-Cl	109.8(5)	C(1)-Hg-N(4)	69.4(8)
N(1)-Hg-N(4)	100.4(6)		

Symmetry transformations used to generate equivalent atoms:

Table S11. Crystal data and structure refinement for **3a.**

Empirical formula	$C_{18}H_{18}B_2F_8HgN_6$	
Formula weight	692.59	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 8.7365(6) Å	α = 90°.
	b = 20.9783(15) Å	β = 97.131(5)°.
	c = 12.9687(10) Å	γ = 90°.
Volume	2358.5(3) $Å^3$	
Z	4	
Density (calculated)	1.951 Mg/m^3	
Absorption coefficient	6.608 mm^{-1}	
F(000)	1320	
Crystal size	0.32 x 0.28 x 0.10 mm^3	
Theta range for data collection	1.857 to 24.983°.	
Index ranges	-10<=h<=9, -24<=k<=24, -14<=l<=15	
Reflections collected	12493	
Independent reflections	3766 [R(int) = 0.0530]	
Completeness to theta = 24.983°	98.3 %	
Absorption correction	multi-scan SADABS	
Max. and min. transmission	0.558 and 0.226	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3766 / 261 / 316	
Goodness-of-fit on F^2	1.060	
Final R indices [I>2sigma(I)]	R1 = 0.0550, wR2 = 0.1231	
R indices (all data)	R1 = 0.0786, wR2 = 0.1343	
Largest diff. peak and hole	4.983 and -2.445 e.$Å^{-3}$	

[a] $R_1 = \Sigma||F_o| - |F_c|| / \Sigma|F_o|$.

[b] $wR_2 = \{\Sigma w(F_o^2 - F_c^2)^2 / \Sigma w(F_o^2)^2\}^{1/2}$.

Table S12. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å ^{2}x 10^3) for **3a.**

Atom	x	y	z	U(eq)[a]
C(1)	3449(12)	7769(5)	2920(8)	25(2)
C(2)	3955(15)	6622(6)	3477(11)	44(3)
C(3)	5842(13)	7543(6)	3593(10)	36(3)
C(4)	3984(13)	8924(6)	2729(9)	30(2)
C(5)	4563(16)	9408(6)	3369(11)	45(3)
C(6)	4216(18)	10039(7)	3082(14)	61(4)
C(7)	3274(18)	10152(7)	2165(13)	62(4)
C(8)	2721(16)	9659(6)	1531(12)	53(3)
C(9)	3113(14)	9041(6)	1808(10)	37(3)
C(10)	-1162(12)	7793(5)	1801(8)	20(2)
C(11)	-1752(15)	6658(5)	1213(11)	43(3)
C(12)	-3491(14)	7612(6)	1067(9)	32(2)
C(13)	-1574(13)	8951(5)	2089(10)	30(2)
C(14)	-1980(17)	9459(6)	1431(12)	53(4)
C(15)	-1590(2)	10066(7)	1789(14)	71(5)
C(16)	-851(19)	10149(7)	2765(13)	68(4)
C(17)	-443(18)	9642(7)	3407(13)	62(4)
C(18)	-850(14)	9039(6)	3059(11)	39(3)
B(1)	2743(17)	8269(7)	5477(12)	37(3)
B(2)	9616(16)	6743(7)	4291(11)	32(2)
N(1)	4380(11)	7293(4)	3311(7)	32(2)
N(2)	5858(10)	8135(5)	3446(7)	34(2)
N(3)	4375(10)	8280(4)	3034(7)	26(19)
N(4)	-2110(11)	7334(4)	1407(7)	28(2)
N(5)	-3503(11)	8221(5)	1259(7)	35(2)
N(6)	-2015(10)	8326(4)	1724(7)	26(19)
F(1)	3006(9)	7624(3)	5324(7)	57(2)
F(2)	1871(8)	8331(3)	6289(6)	46(18)
F(3)	1955(10)	8525(4)	4589(6)	65(2)
F(4)	4156(8)	8562(4)	5726(7)	59(2)
F(5)	10368(9)	6653(3)	3407(6)	49(19)
F(6)	9363(8)	7390(3)	4400(6)	48(19)
F(7)	8205(8)	6438(3)	4148(6)	55(2)
F(8)	10514(9)	6499(4)	5142(6)	61(2)
Hg	1149(5)	7749(2)	2372(3)	24(18)

[a] U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Table S13. Anisotropic displacement parameters ($Å^2 x 10^3$) for **3a.**

Atom	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C(1)	18(4)	35(4)	23(5)	6(3)	8(3)	3(4)
C(2)	36(7)	43(5)	52(9)	9(4)	6(6)	7(5)
C(3)	17(4)	50(5)	39(7)	10(3)	-1(4)	2(4)
C(4)	21(5)	35(4)	36(5)	0(3)	7(4)	4(3)
C(5)	47(7)	41(5)	48(6)	-7(4)	5(6)	-1(4)
C(6)	68(9)	41(6)	74(8)	-4(5)	13(7)	3(5)
C(7)	65(9)	41(6)	79(8)	-4(5)	12(7)	11(5)
C(8)	49(8)	44(5)	66(8)	-1(5)	10(6)	17(5)
C(9)	32(6)	38(5)	40(6)	-6(4)	4(5)	8(4)
C(10)	20(4)	25(4)	18(5)	-7(3)	9(3)	6(3)
C(11)	44(7)	32(5)	51(8)	-3(4)	-1(7)	-6(5)
C(12)	28(5)	46(5)	22(6)	-6(3)	9(4)	-3(4)
C(13)	19(5)	29(4)	44(5)	2(4)	8(4)	-2(4)
C(14)	64(9)	34(5)	60(7)	7(5)	1(6)	4(4)
C(15)	87(11)	37(6)	88(9)	3(6)	7(8)	-2(5)
C(16)	76(11)	39(6)	88(8)	1(6)	10(7)	-14(5)
C(17)	66(9)	44(6)	76(8)	-4(5)	4(7)	-21(5)
C(18)	33(7)	34(5)	48(6)	6(4)	-1(5)	-9(4)
B(1)	31(5)	42(5)	39(5)	3(4)	12(4)	3(4)
B(2)	35(5)	31(5)	32(5)	4(4)	7(4)	1(4)
N(1)	24(4)	41(4)	30(5)	8(3)	6(4)	5(4)
N(2)	12(4)	56(5)	33(5)	1(3)	2(4)	9(4)
N(3)	15(4)	38(4)	28(5)	4(3)	7(3)	2(3)
N(4)	25(4)	31(4)	28(5)	-7(3)	5(4)	1(3)
N(5)	26(4)	46(4)	31(5)	-3(3)	2(4)	0(4)
N(6)	23(4)	29(3)	25(5)	0(3)	5(3)	4(3)
F(1)	47(5)	48(4)	73(6)	8(3)	0(4)	-15(3)
F(2)	42(4)	51(4)	47(4)	6(3)	19(3)	6(3)
F(3)	62(5)	83(6)	49(4)	14(4)	7(4)	18(4)
F(4)	38(4)	52(4)	89(6)	-5(3)	10(4)	2(4)
F(5)	58(5)	48(4)	45(4)	11(3)	20(4)	5(3)
F(6)	44(4)	37(4)	62(5)	7(3)	1(4)	-10(3)
F(7)	41(4)	49(4)	75(6)	-6(3)	6(4)	3(4)
F(8)	57(5)	80(5)	45(4)	14(4)	1(4)	17(4)
Hg	20(3)	23(2)	29(3)	1(19)	3(18)	1(2)

Table S14. Hydrogen coordinates ($x\ 10^4$) and isotropic displacement parameters ($Å^2 x\ 10^3$) for **3a.**

Atom	x	y	z	U(eq)
H(2A)	4871	6384	3772	66
H(2B)	3174	6606	3957	66
H(2C)	3537	6431	2811	66
H(3)	6717	7299	3862	43
H(5)	5194	9317	4002	54
H(6)	4621	10382	3509	73
H(7)	3004	10578	1971	74
H(8)	2071	9743	903	64
H(9)	2775	8699	1356	44
H(11A)	-2695	6438	917	65
H(11B)	-983	6635	725	65
H(11C)	-1342	6454	1869	65
H(12)	-4352	7386	727	38
H(14)	-2510	9393	755	64
H(15)	-1838	10425	1353	85
H(16)	-611	10569	3008	81
H(17)	110	9706	4077	75
H(18)	-622	8682	3504	47

Table S15. Bond lengths [Å] and angles [°] for **3a.**

Bond lengths			
C(1)-N(3)	1.339(14)	C(17)-C(18)	1.376(17)
C(1)-N(1)	1.347(13)	C(6)-C(7)	1.380(2)
C(1)-Hg	2.047(11)	C(7)-C(8)	1.370(2)
C(12)-N(5)	1.301(15)	B(1)-F(3)	1.376(16)
C(2)-N(1)	1.478(15)	B(1)-F(2)	1.380(16)
C(12)-N(4)	1.364(15)	C(8)-C(9)	1.375(17)
C(13)-C(18)	1.349(18)	B(1)-F(4)	1.381(16)
C(13)-C(14)	1.383(17)	B(1)-F(1)	1.391(16)
C(3)-N(2)	1.257(15)	B(2)-F(8)	1.371(15)
C(13)-N(6)	1.431(14)	C(10)-N(4)	1.330(13)
C(3)-N(1)	1.387(15)	B(2)-F(7)	1.381(16)
C(14)-C(15)	1.383(19)	C(10)-N(6)	1.340(13)
C(4)-C(9)	1.357(15)	B(2)-F(6)	1.385(15)
C(15)-C(16)	1.360(2)	C(10)-Hg	2.064(10)
C(4)-C(5)	1.368(17)	B(2)-F(5)	1.404(15)
C(4)-N(3)	1.438(14)	C(11)-N(4)	1.480(14)
C(16)-C(17)	1.370(2)	N(2)-N(3)	1.373(12)
C(5)-C(6)	1.396(18)	N(5)-N(6)	1.381(12)
Angles			
N(3)-C(1)-N(1)	102.9(9)	C(7)-C(8)-C(9)	119.7(14)
C(14)-C(13)-N(6)	117.7(12)	F(7)-B(2)-F(6)	108.5(10)
N(3)-C(1)-Hg	127.5(8)	F(8)-B(2)-F(5)	109.1(10)
C(15)-C(14)-C(13)	117.9(15)	F(7)-B(2)-F(5)	109.2(11)
N(1)-C(1)-Hg	129.5(8)	C(4)-C(9)-C(8)	119.6(13)
C(16)-C(15)-C(14)	120.0(15)	F(6)-B(2)-F(5)	108.2(10)
C(15)-C(16)-C(17)	121.6(14)	C(1)-N(1)-C(3)	108.2(10)
N(2)-C(3)-N(1)	111.2(10)	C(1)-N(1)-C(2)	127.6(10)
C(16)-C(17)-C(18)	118.6(15)	N(4)-C(10)-N(6)	105.2(9)
C(9)-C(4)-C(5)	121.6(11)	C(3)-N(1)-C(2)	124.2(10)
C(9)-C(4)-N(3)	120.0(11)	N(4)-C(10)-Hg	129.8(8)
C(13)-C(18)-C(17)	120.2(13)	C(3)-N(2)-N(3)	104.4(10)
C(5)-C(4)-N(3)	118.3(11)	N(6)-C(10)-Hg	125.0(7)
C(4)-C(5)-C(6)	119.3(14)	C(1)-N(3)-N(2)	113.2(9)
F(3)-B(1)-F(2)	109.6(11)	C(1)-N(3)-C(4)	127.0(9)
F(3)-B(1)-F(4)	111.2(11)	N(2)-N(3)-C(4)	119.7(9)
C(7)-C(6)-C(5)	118.6(15)	C(10)-N(4)-C(12)	107.3(9)
F(2)-B(1)-F(4)	110.0(12)	C(10)-N(4)-C(11)	128.6(10)
F(3)-B(1)-F(1)	109.5(12)	C(12)-N(4)-C(11)	123.5(10)
F(2)-B(1)-F(1)	108.5(11)	C(12)-N(5)-N(6)	102.2(9)
C(8)-C(7)-C(6)	121.0(14)	N(5)-C(12)-N(4)	112.7(10)
F(4)-B(1)-F(1)	107.9(11)	C(10)-N(6)-N(5)	112.5(9)
F(8)-B(2)-F(7)	110.3(11)	C(10)-N(6)-C(13)	128.0(9)
F(8)-B(2)-F(6)	111.5(11)	N(5)-N(6)-C(13)	119.4(9)

C(18)-C(13)-C(14)	121.7(11)	C(18)-C(13)-N(6)	120.5(11)
C(1)-Hg-C(10)	176.2(4)		

Symmetry transformations used to generate equivalent atoms: