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Supplementary Data

Syntheses,crystal structures and antimicrobial activities of copper(II), ruthenium(II) and platinum(II) compounds of anthracene-containing tripodal ligand

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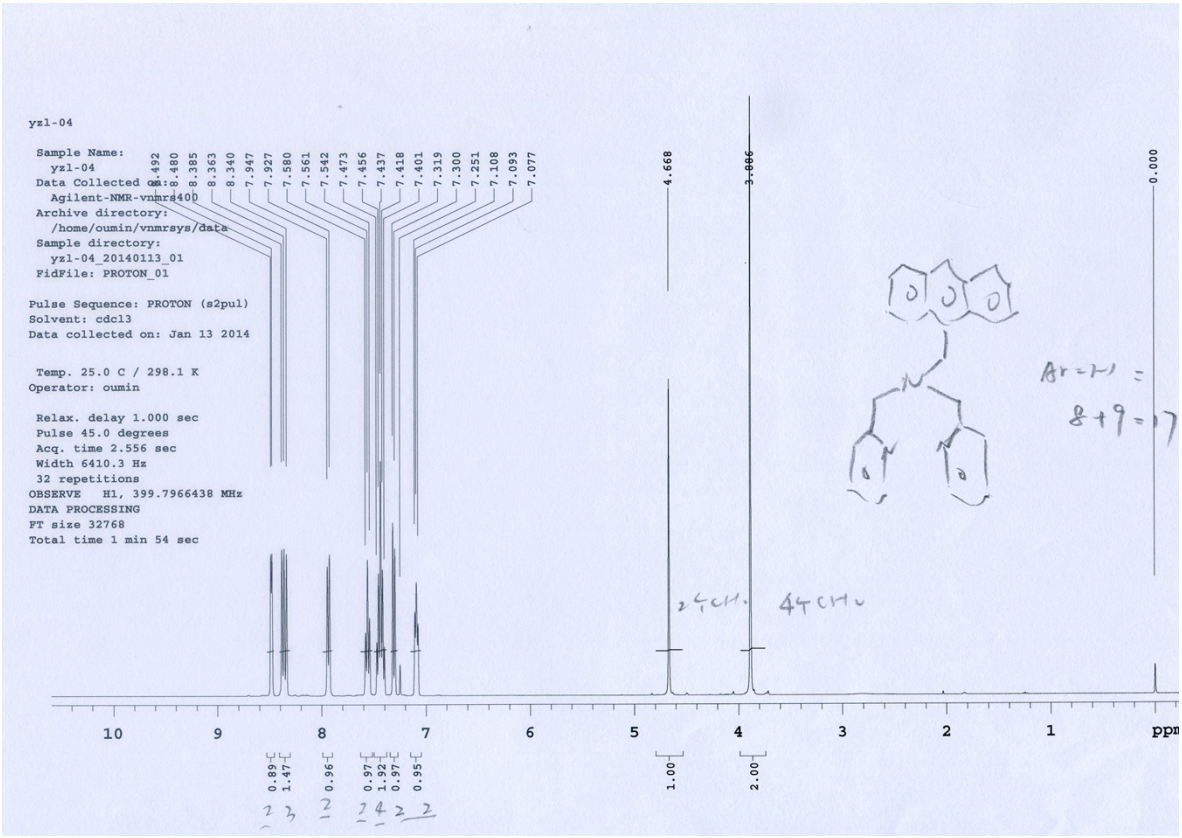

Fig. S1 ^{1}H NMR of ADPA

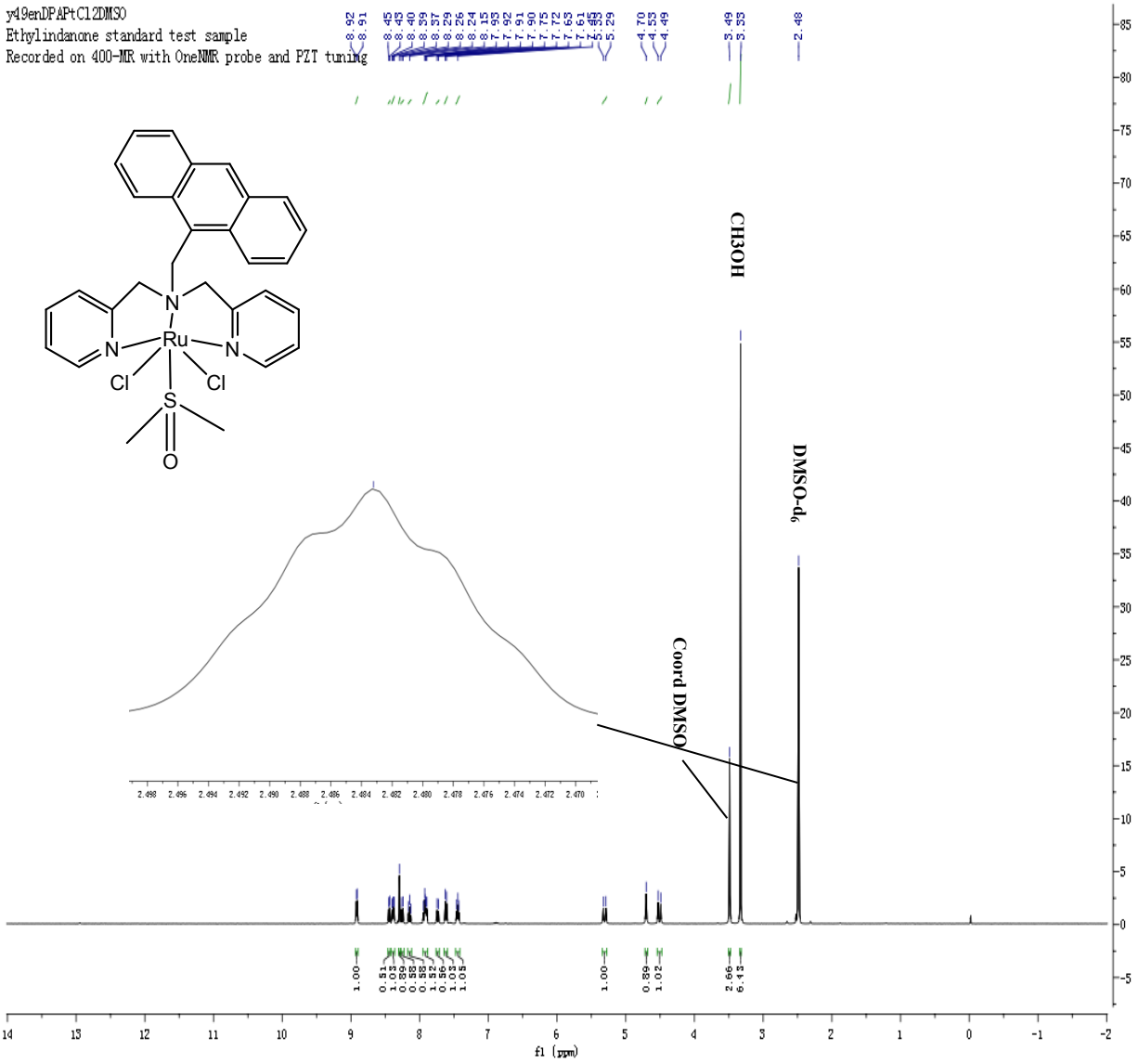

Fig. S2 ^{1}H NMR of compound **2**(Insert :magnify for DMSO-d_6 peak at 2.47 to 2.50 ppm. Non-coord DMSO peak has not been found at 2.52 ppm)

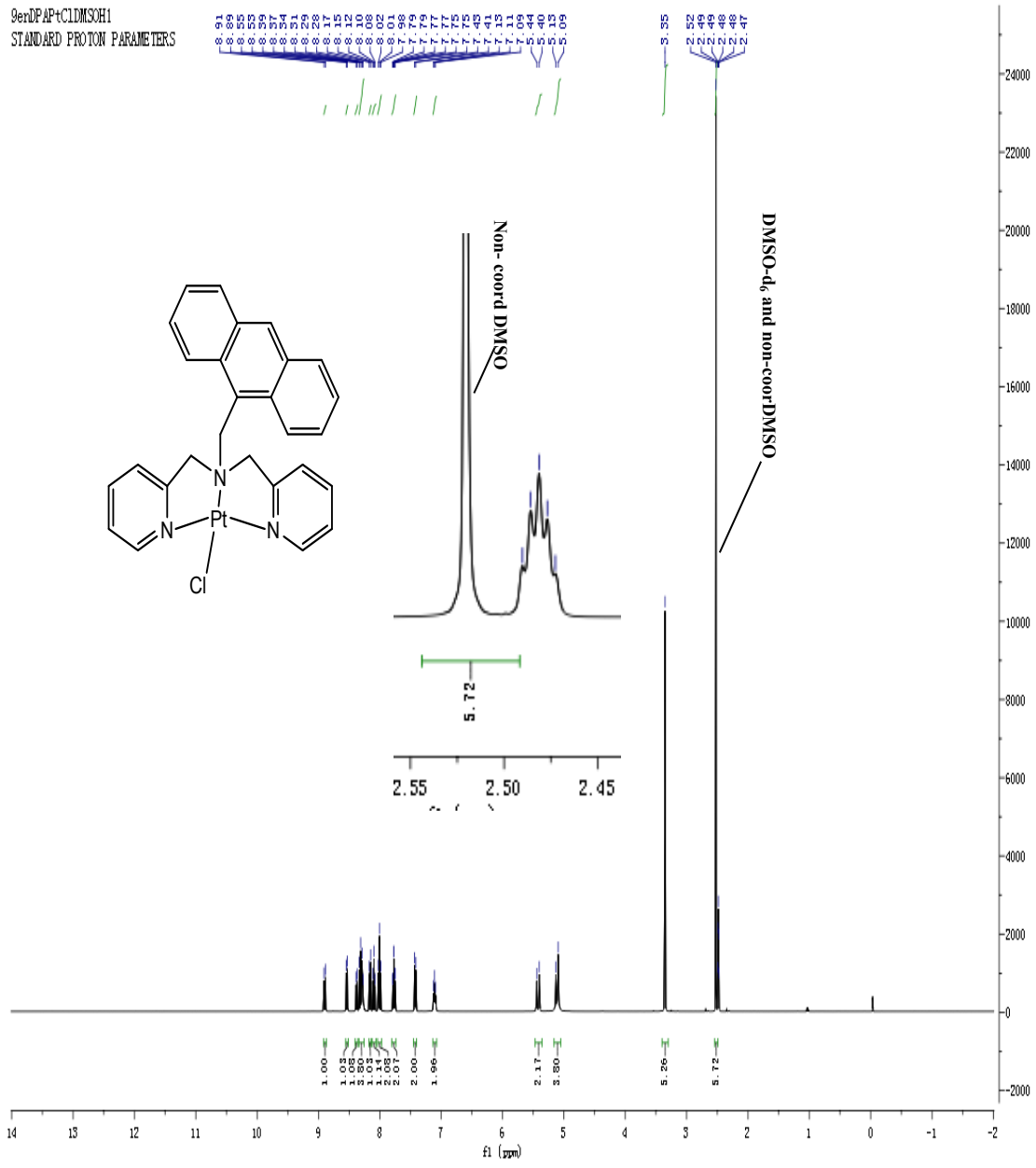

Fig. S3 ^{1}H NMR of compound **3** (Insert :magnify for peak at 2.49 ppm. Non-coord DMSO peak has been found at 2.52 ppm)

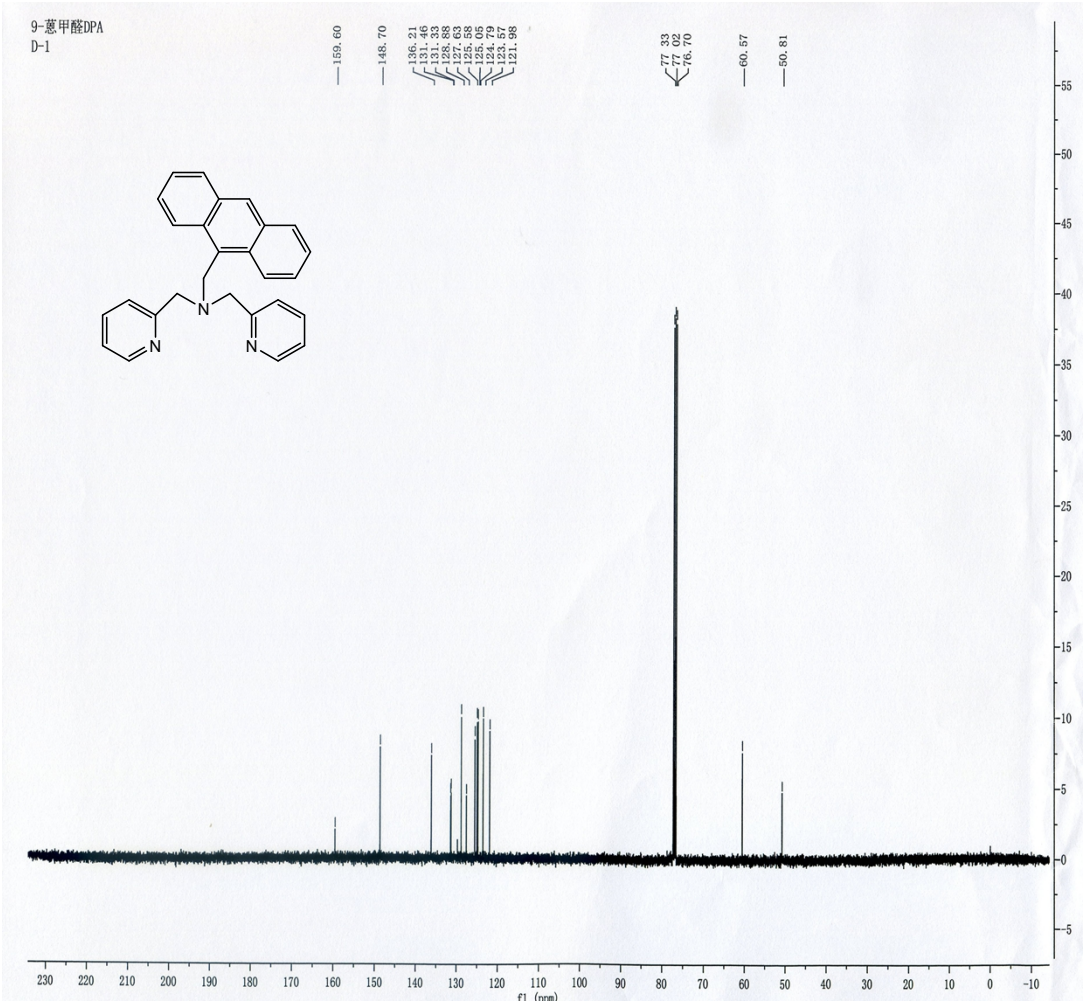

Fig. S4 ^{13}C NMR of ADPA

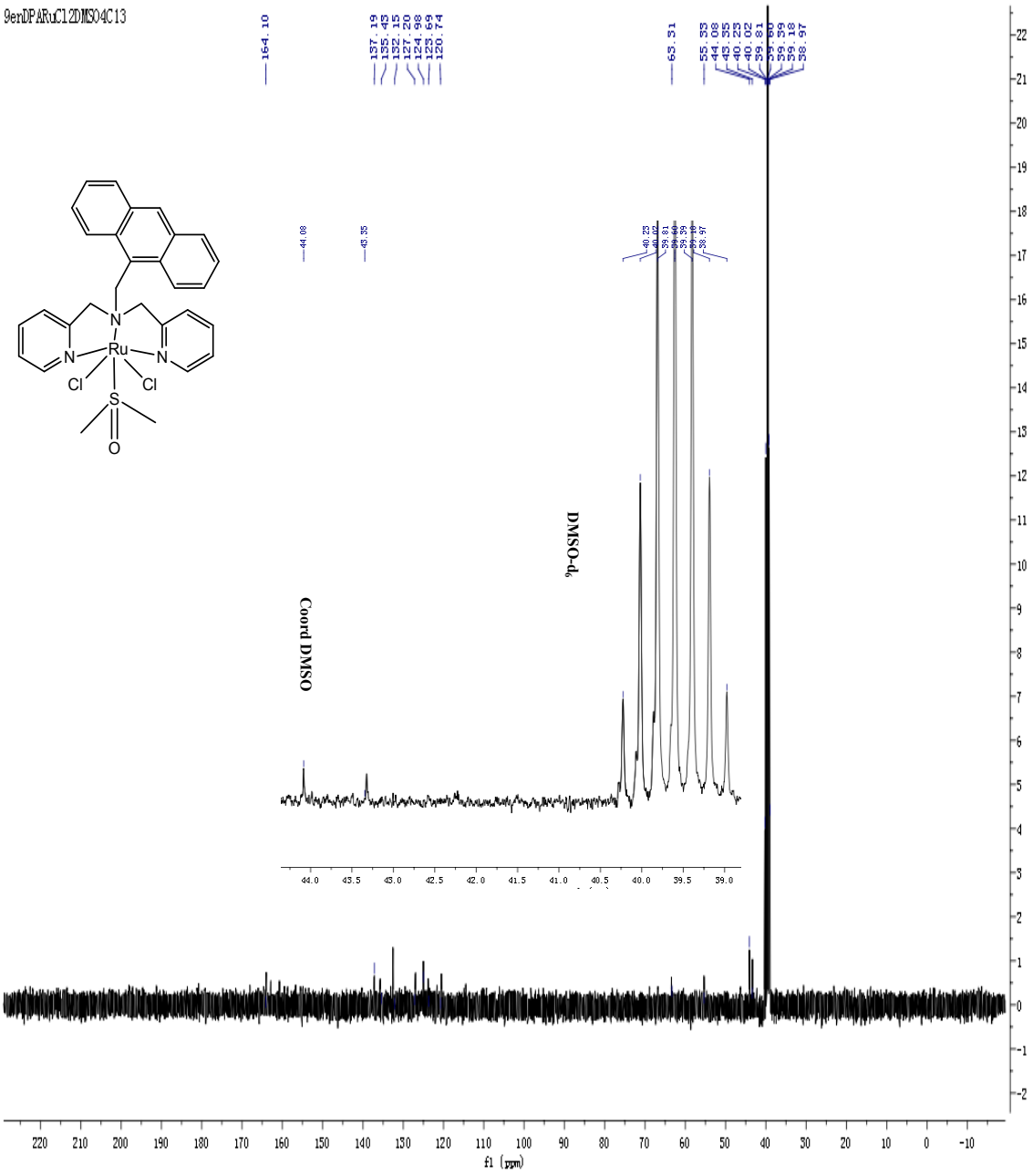

Fig. S5 ^{13}C NMR of compound **2** (Insert :magnify for peak at 39.0 to 44.5 ppm. coord DMSO peak has been found at 44.08 ppm.)

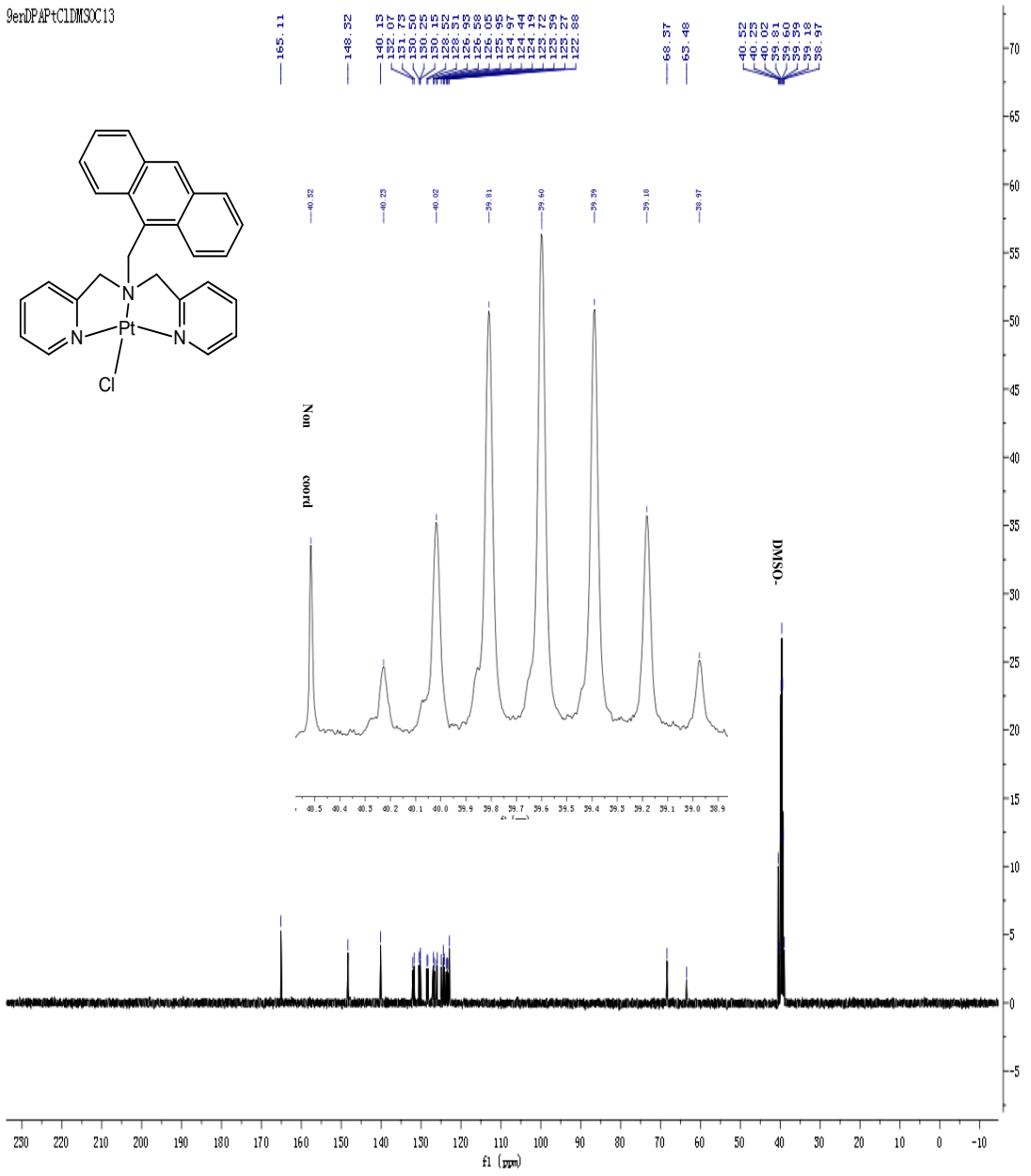

Fig. S6 ^{13}C NMR of compound **3** (Insert :magnify for peak at 39.0 to 41.0 ppm. Non- coord DMSO peak has been found at 40.52 ppm)

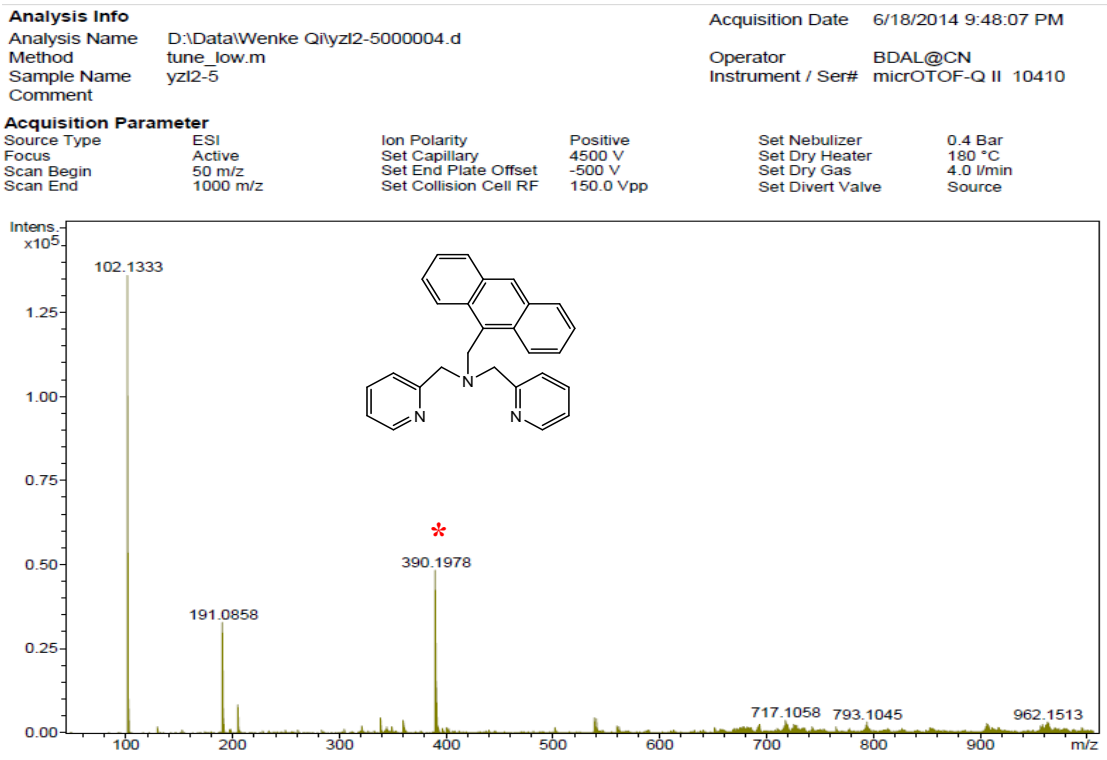

Fig. S7 H RMS of ADPA .

The parent ion peaks at *m/z* 390.1978 is marked with asterisks.

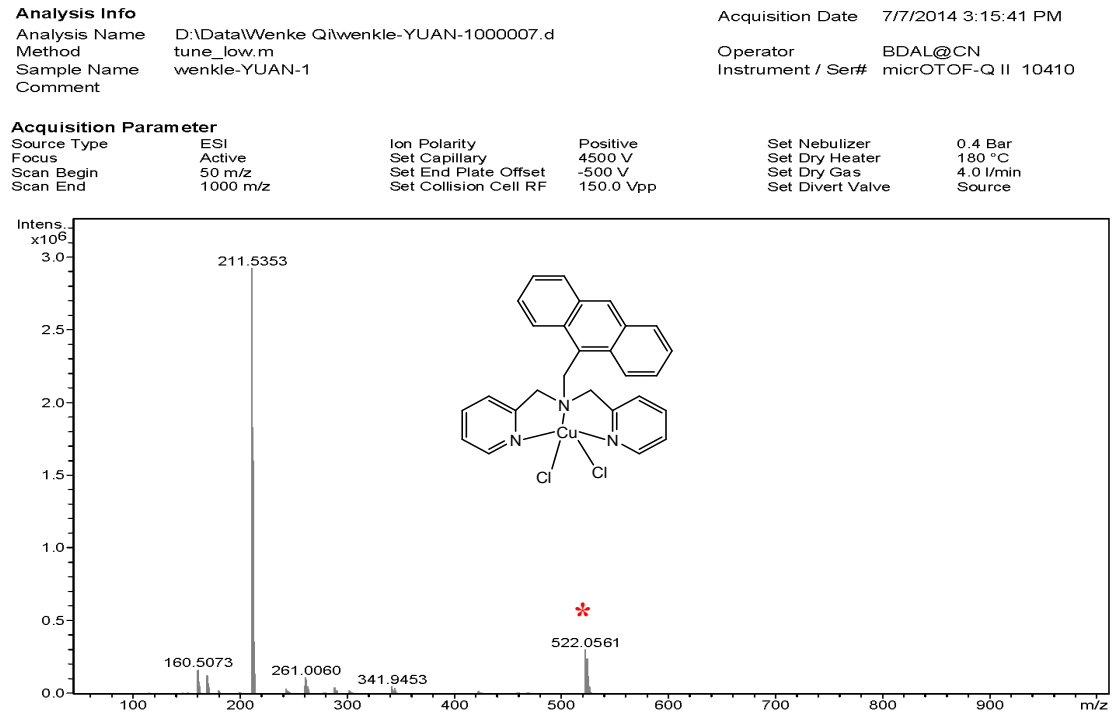

Fig. S8 H RMS of compound **1** .

The parent ion peaks at *m/z* 522.0561 is marked with asterisks.

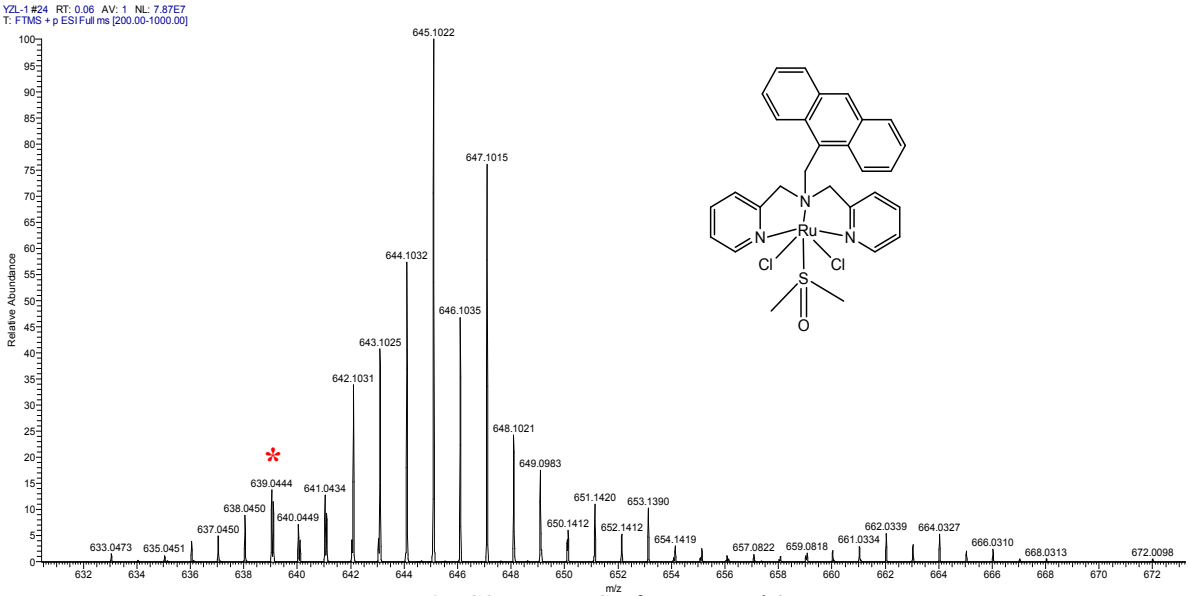

Fig. S9 H RMS of compound **2** .

The cationic fragment peaks at m/z 639.0444 is marked with asterisks.

Fig. S10 H RMS of compound **3** .

The cationic fragment peaks at m/z 619.1207 is marked with asterisks.

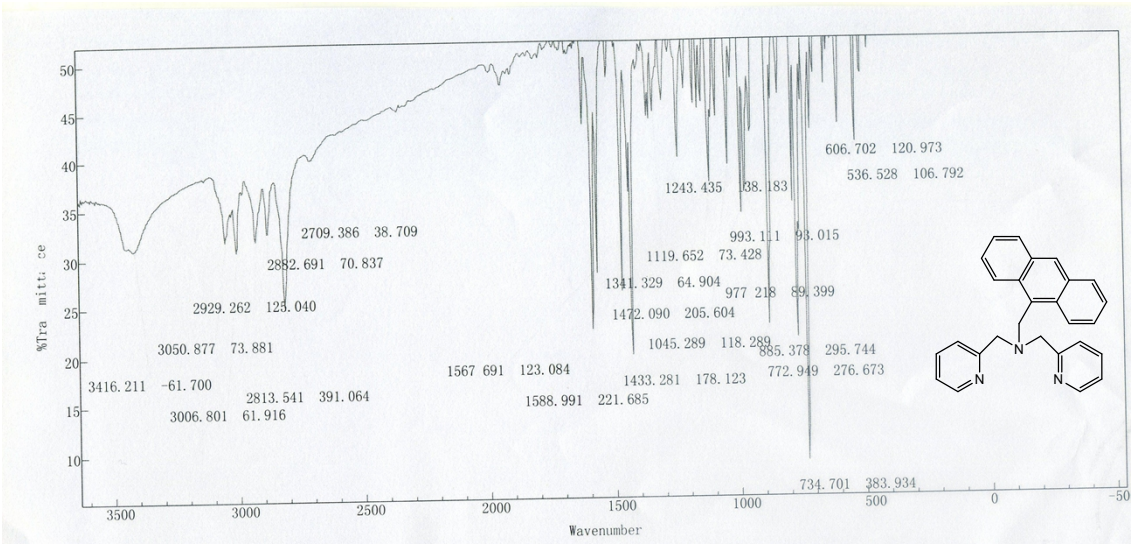

Fig. S11 FT-IR of ADPA

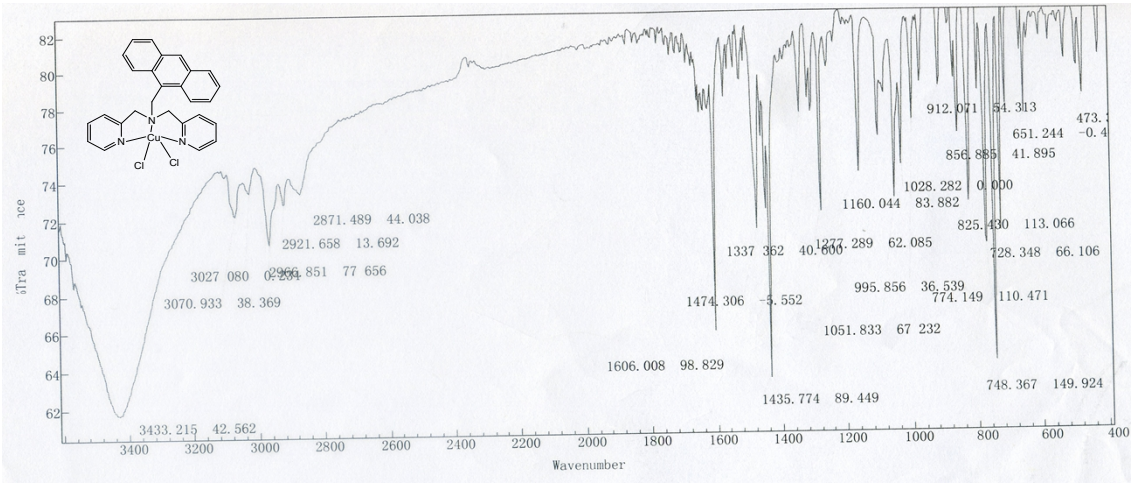

Fig. S12 FT-IR of compound **1**

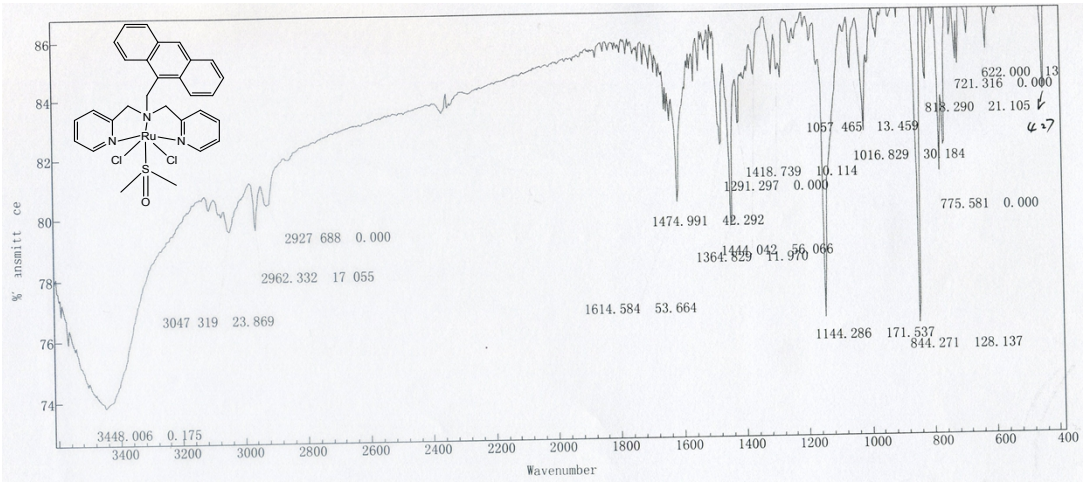

Fig. S13 FT-IR of compound

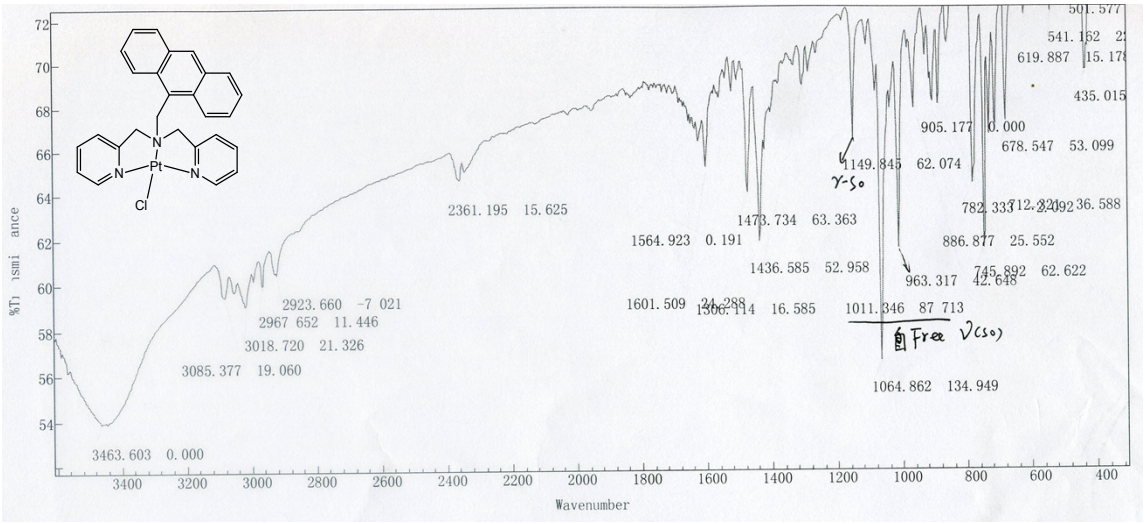

Fig. S14 FT-IR of compound 3

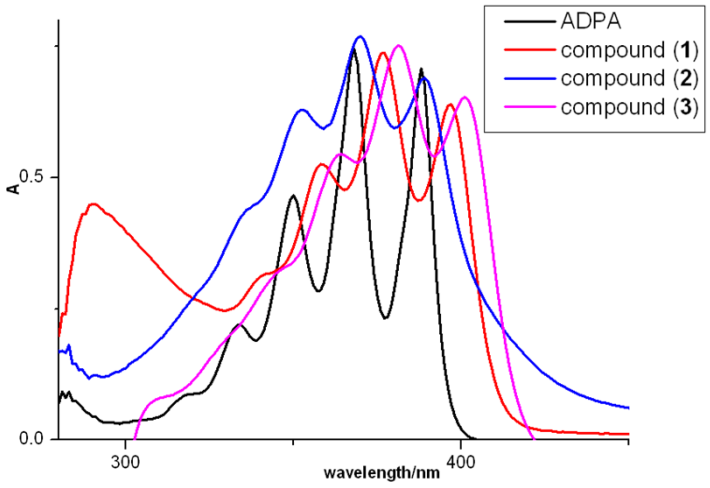

Fig. S15 UV-vis of liand(ADPA)and compounds 1-3

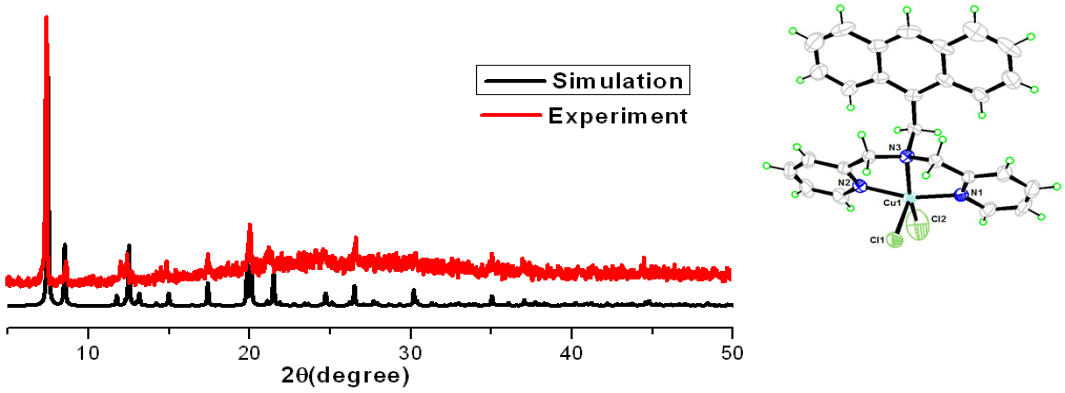

Fig. S16 The simulated and experimental PXRD patterns of compound **1**

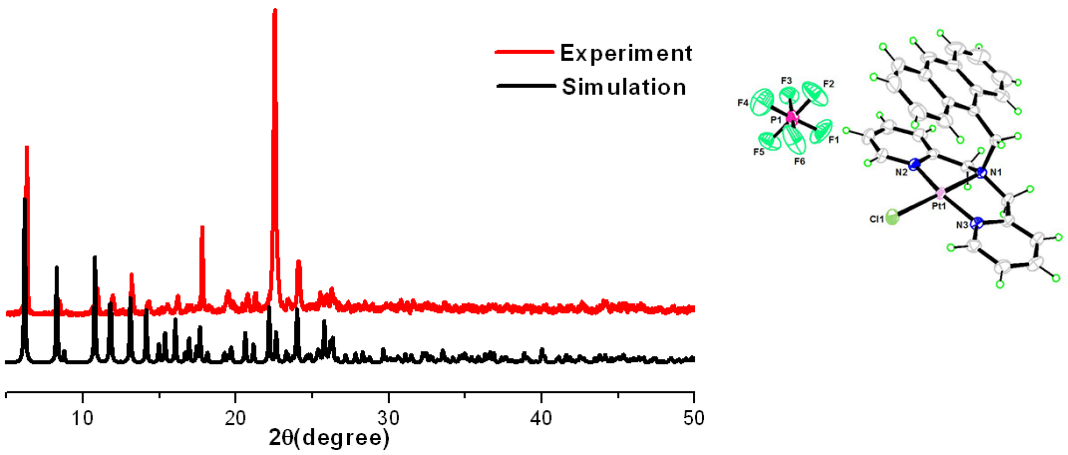

Fig. S17 The simulated and experimental PXRD patterns of compound **3**

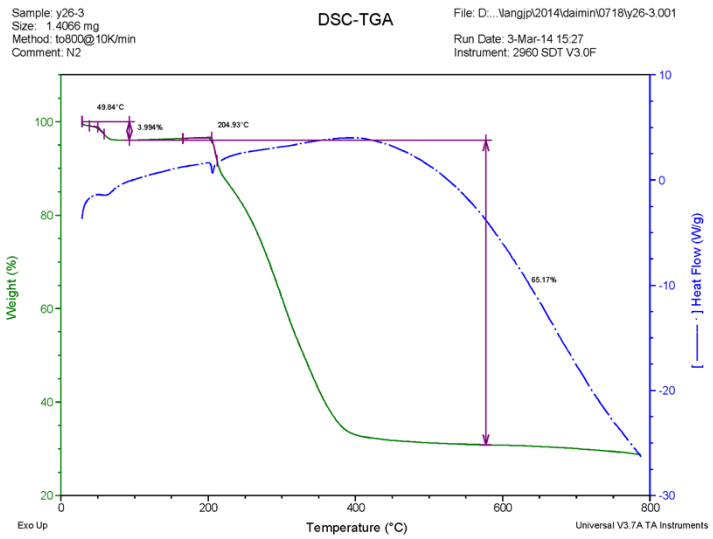

Fig. S18 TG curves of compound **1**

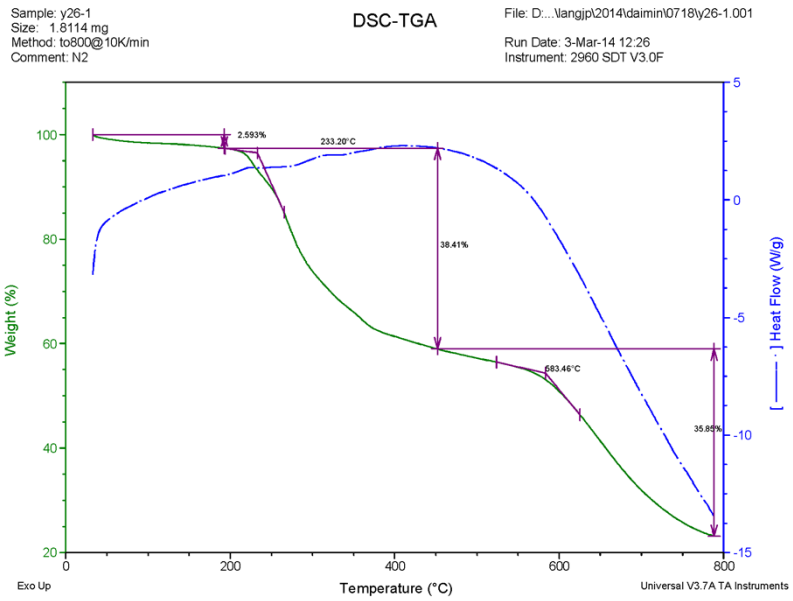

Fig. S19 TG curves of compound **2**

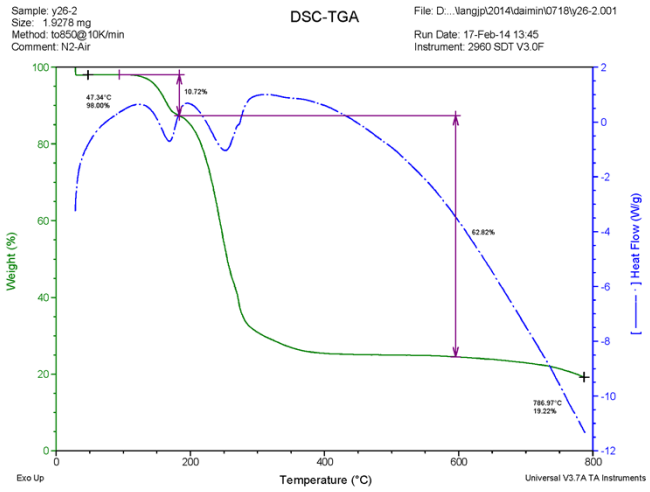

Fig. S20 TG curves of compound **3**

Table S1 Pertinent Crystal Data and Structure Refinement Results for Compounds **1**−**3**

Compounds	**1**	**2**	**3**
Formula	$CuC_{27}N_3H_{23}Cl_2O$	$C_{29}H_{28}ON_3Cl_2RuS$	$PtC_{27}N_3H_{23}ClPF_6$
Mr	541.94	639.58	764.98
Space group	*Pna2(1)*	*R-3*	*P-1*
a (Å)	20.6261(8)	25.875(4)	8.2692(3)
b (Å)	14.7505(6)	25.875(4)	11.1553(4)
c (Å)	8.7896(3)	25.597(4)	14.9524(6)
α (deg)	90	90	72.155(1)
β (deg)	90	90	81.810(1)
γ (deg)	90	120	83.298(1)
V (Å^3)	2674.20(18)	14842(6)	1295.63(8)
Z	4	18	2
D_c (g cm^{-3})	1.341	1.288	1.961
M (mm^{-1})	1.040	0.724	5.647
F(000)	1116.0	5868.0	740.0
GOF	1.171	1.014	1.033
R_1[a]	0.0392	0.0450	0.0257
wR_2[a]	0.1438	0.0987	0.0676

[a] $R_1 = \sum (||Fo| - |Fc||)/\sum |Fo|$, $wR = \{\sum w[(Fo^2 - Fc^2)^2]/\sum w[(Fo2)^2]\}^{1/2}$

Table S2. Selected bond lengths (Å) and angles (º) for Compound **1**

Cu1—N1	2.005(3)	C13—C14	1.419(5)
Cu1—N2	2.008(3)	C13—C15	1.522(6)
Cu1—N3	2.091(3)	C15—N3	1.509(5)
Cu1—Cl2	2.2572(13)	C16—C17	1.506(6)
Cu1—Cl1	2.4855(15)	C17—N1	1.332(6)
C1—N3	1.508(6)	C17—C18	1.392(6)
C1—C2	1.354(6)	C18—C19	1.408(8)
C1— C14	1.425(6)	C19—C20	1.371(8)
C2—C3	1.408(9)	C20—C21	1.368(7)
C3—C4	1.335(8)	C21—N1	1.336(6)
C4—C5	1.429(7)	C22—N3	1.479(5)
C5—C6	1.420(7)	C22—C23	1.528(6)
C6—C7	1.377(6)	C23—N2	1.333(6)
C7—C8	1.411(7)	C23—C24	1.385(6)
C8—C9	1.357(8)	C24—C25	1.383(8)
C7—C12	1.440(7)	C25—C27	1.348(9)
C9—C10	1.417(9)	C26—C27	1.366(8)
C10—C11	1.362(6)	C26—N2	1.345(6)
C11—C12	1.420(6)		
C12—C13	1.423(5)		
N1—Cu1—N2	161.18(14)	C14—C13—C15	120.2(3)
N1—Cu1—N3	81.13(12)	C12—C13—C15	120.3(3)
N2—Cu1—N3	80.93(13)	N3—C15—C13	115.9(4)
N1—Cu1—Cl2	96.56(12)	N3—C16—C17	109.5(4)
N2—Cu1—Cl2	97.41(12)	C18—C17-C16	122.0(4)
N3—Cu1—Cl2	155.60(11)	C17—C18—C19	117.6(5)
N1—Cu1—Cl1	93.34(13)	C20—C19—C18	119.5(4)
N2—Cu1—Cl1	94.00(13)	C21—C20—C19	118.9(5)
N3—Cu1—Cl1	95.51(11)	N1—C17—C18	121.9(4)
Cl2—Cu1—Cl1	108.89(7)	N1—C17—C16	116.1(3)
C2—C1—C14	122.5(5)	N1—C21—C20	122.5(5)
C1—C2—C3	120.6(5)	C24—C23—C22	122.8(4)
C4—C3—C2	120.0(5)	C25—C24—C23	118.0(5)

C3—C4—C5	121.2(5)	C27—C25—C24	120.5(5)
C6—C5—C14	118.6(4)	C25—C26—C27	119.7(6)
C6—C5—C4	121.6(5)	N2—C26—C27	122.1(5)
C14—C5—C4	119.8(5)	C17—N1—C21	119.6(4)
C7—C6—C5	121.9(5)	C17—N1—Cu1	113.5(3)
C6—C7—C12	119.8(4)	C21—N1—Cu1	126.9(3)
C8—C7—C12	120.4(4)	C23—N2—C26	119.0(4)
C6—C7—C8	119.8(5)	C23—N2—Cu1	113.7(3)
C9—C8—C7	120.5(5)	C26—N2—Cu1	127.2(3)
N3— C22—C23	109.2(3)	C16—N3—C15	113.6(3)
C1—C14—C5	115.7(4)	C22—N3—C15	113.8(3)
C8—C9—C10	120.0(5)	C16—N3—C11	104.2(2)
C11—C10—C9	120.7(5)	C22—N3—Cu1	104.2(2)
C13—C14—C1	124.3(4)	C15—N3—Cu1	107.4(3)
C13—C14—C5	120.1(4)	C1—N3—Cu1	107.1(3)
C11—C12—C13	123.6(4)		
C11—C12—C7	116.7(4)		
C13—C12—C7	119.7(4)		
C14—C13—C12	119.5(4)		

Table S3. Selected bond lengths (Å) and angles (º) for Compound **2**

Ru1—N3	2.077(3)	C16—H16A	0.9700
Ru1—N2	2.097(3)	C16—H16B	0.9700
Ru1—N1	2.142(3)	C17—N2	1.349(5)
Ru1—S1	2.2284(12)	C17—C18	1.381(5)
Ru1—Cl2	2.4227(11)	C18—C19	1.380(6)
Ru1—Cl1	2.4350(11)	C18—H18A	0.9300
C1—C14	1.415(5)	C19—C20	1.362(6)
C1—C2	1.419(6)	C19—H19A	0.9300
C1—C6	1.437(6)	C20—C21	1.374(6)
C2—C3	1.366(6)	C20—H20A	0.9300
C2—H2A	0.9300	C21—N2	1.338(5)
C3—C4	1.413(8)	C21—H21A	0.9300
C3—H3A	0.9300	C22—C23	1.479(5)
C4—C5	1.316(7)	C22—N1	1.492(4)
C4—H4A	0.9300	C22—H22A	0.9700

C5—C6	1.416(6)	C22—H22B	0.9700
C5—H5A	0.9300	C23—N3	1.355(5)
C6—C7	1.381(6)	C23—C24	1.380(5)
C7—C8	1.378(6)	C24—C25	1.374(6)
C7—H7A	0.9300	C24—H24A	0.9300
C8—C13	1.428(6)	C25—C26	1.373(6)
C8—C9	1.444(6)	C25—H25A	0.9300
C9—C10	1.340(7)	C26—C27	1.360(6)
C9—H9A	0.9300	C26—H26A	0.9300
C10—C11	1.394(7)	C27—N3	1.347(5)
C10—H10A	0.9300	C27—H27A	0.9300
C11—C12	1.344(6)	C28—S1	1.783(4)
C11—H11A	0.9300	C28—H28A	0.9600
C12—C13	1.441(6)	C28—H28B	00.9600
C12—H12A	0.9300	C28—H28C	0.9600
C13—C14	1.406(5)	C29—S1	1.785(5)
C14—C15	1.534(5)	C29—H29A	0.9600
C15—N1	1.511(4)	C29—H29B	0.9600
C15—H15A	0.9500	C29—H29C	0.9600
C16—C17	1.47 (5)	O1—S1	1.483(3)
C16—N1	1.507(4)		

N3—Ru1—N2	95.11(12)	N2—C17—C18	121.7(4)
N3—Ru1—N1	78.25(12)	N2—C17—C16	114.7(3)
N2—Ru1—N1	80.83(11)	C18—C17—C16	123.5(4)
N3—Ru1—S1	91.64(9)	C17—C18—C19	119.2(4)
N2—Ru1—S1	172.94(9)	C17—C18—H18A	120.4
N1—Ru1—S1	98.55(8)	C19—C18—H18A	120.4
N3—Ru1—Cl2	93.84(9)	C20—C19—C18	119.1(4)
N2—Ru1—Cl2	93.32(9)	C20—C19—H19A	120.4
N1—Ru1—Cl2	169.61(8)	C18—C19—H19A	120.4
S1—Ru1—Cl2	88.30(4)	C21—C20—C19	119.1(4)
N3—Ru1—Cl1	174.73(9)	C21—C20—H20A	120.84
N2—Ru1—Cl1	83.03(9)	C19—C20—H20A	120.4
N1—Ru1—Cl1	96.57(8)	N2—C21—C20	122.8(4)
S1—Ru1—Cl1	90.07(4)	N2—C21—H21A	118.6
Cl2—Ru1—Cl1	91.19(4)	C20—C21—H21A	118.6
C14—C1—C2	123.9(4)	C23—C22—N1	109.6(3)
C14—C1—C6	119.3(4)	C23—C22—H22A	109.7
C2—C1—C6	116.8(4)	N1—C22—H22A	109.7

C3—C2—C1	121.6(5)	C23—C22—H22B	109.7
C3—C2—H2A	119.2	N1—C22—H22B	109.7
C1—C2—H2A	119.2	H22A—C22—H22B	108.2
C2—C3—C4	120.3(5)	N3—C23—C24	121.0(4)
C2—C3—H3A	119.9	N3—C23—C22	115.6(3)
C4—C3—H3A	119.9	C24—C23—C22	123.4(4)
C5—C4—C3	120.0(5)	C23—C24—C25	119.1(4)
C5—C4—H4A	120.0	C23—C24—H24A	120.4
C3—C4—H4A	120.0	C25—C24—H24A	120.4
C4—C5—C6	122.6(5)	C26—C25—C24	119.5(4)
C4—C5—H5A	118.7	C26—C25—H25A	120.3
C6—C5—H5A	118.7	C24—C25—H25A	120.3
C7—C6—C5	122.5(5)	C25—C26—C27	119.5(4)
C7—C6—C1	118.6(4)	C25—C26—H26A	120.2
C5—C6—C1	118.8(5)	C27—C26—H26A	120.2
C8—C7—C6	123.1(4)	N3—C27—C26	121.8(4)
C6—C7—H7A	118.4	N3—C27—H27A	119.1
C8—C7—H7A	118.4	C26—C27—H27A	119.1
C7—C8—C13	119.1(4)	S1—C28—H28A	109.5
C7—C8—C9	121.6(5)	S1—C28—H28B	109.5
C13—C8—C9	119.1(5)	H28A—C28—H28B	109.5
C10—C9—C8	120.3(5)	S1—C28—H28C	109.5
C10—C9—H9A	119.9	H28A—C28—H28C	109.5
C8—C9—H9A	119.9	H28B—C28—H28C	109.5
C9—C10—C11	121.2(5)	S1—C29—H29A	109.5
C9—C10—H10A	119.4	S1—C29—H29B	109.5
C11—C10—H10A	119.4	H29A—C29—H29B	109.5
C12—C11—C10	121.0(5)	S1—C29—H29C	109.5
C12—C11—H11A	119.5	H29A—C29—H29C	109.5
C10—C11—H11A	119.5	H29B—C29—H29C	109.5
C11—C12—C13	121.6(4)	C22—N1—C15	112.9(3)
C11—C12—H12A	119.2	C22—N1—C16	106.9(3)
C13—C12—H12A	119.2	C15—N1—C16	113 (3)
C14—C13—C8	119.4(4)	C22—N1—Ru1	104.8(2)

C14—C13—C12	123.8(4)	C15—N1—Ru1	112.4(2)
C8—C13—C12	116.7(4)	C16—N1—Ru1	106.8(2)
C1—C14—C13	120.2(4)	C17—N2—C21	124.9(3)
C1—C14—C15	119.6(4)	C17—N2—Ru1	115 (3)
C13—C14—C15	119.7(3)	C21—N2—Ru1	125 (3)
N1—C15—C14	116.7(3)	C27—N3—C23	119.0(3)
N1—C15—H15A	108.1	C27—N3—Ru1	126.5(3)
C14—C15—H15A	108.1	C23—N3—Ru1	114.4(3)
C17—C16—N1	112.4(3)	C28—S1—C29	29 98.2(2)
C17—C16—H16A	109.1	C28—S1—O1	106.0(2)
N1—C16—H16A	109.1	C29—S1—O1	105.4(2)
C17—C16—H16B	109.1	C28—S1—Ru1	112.25(17)
N1—C16—H16B	109.1	C29—S1—Ru1	112.39(17)
H16A—C16—H16B	107.9	O1—S1—Ru1	120.13(12)

C14—C1—C2—C3	178.3(4)	S1—Ru1—N1—C22	56.1(2)
C6—C1—C2—C3	0.4(6)	Cl2—Ru1—N1—C22	-74.8(5)
C1—C2—C3—C4	-0.1(7)	Cl1—Ru1—N1—C22	147.1(2)
C2—C3—C4—C5	-0.1(8)	N3—Ru1—N1—C15	-156.8(2)
C3—C4—C5—C6	0.1(9)	N2—Ru1—N1—C15	106.0(2)
C4—C5—C6—C7	-176.8(5)	S1—Ru1—N1—C15	-66.9(2)
C4—C5—C6—C1	0.2(8)	Cl2—Ru1—N1—C15	162.3(3)
C14—C1—C6—C7	-1.3(6)	Cl1—Ru1—N1—C15	24.2(2)
C2—C1—C6—C7	176.7(4)	N3—Ru1—N1—C16	79.3(2)
C14—C1—C6—C5	-178.4(4)	N2—Ru1—N1—C16	-17.9(2)
C2—C1—C6—C5	-0.4(6)	S1—Ru1—N1—C16	169.23(19)
C5—C6—C7—C8	176.1(4)	Cl2—Ru1—N1—C16	38.4(6)
C1—C6—C7—C8	-1.0(7)	Cl1—Ru1—N1—C16	-99.7(2)
C6—C7—C8—C13	-0.1(7)	C18—C17—N2—C21	0.1(6)
C6—C7—C8—C9	-176.3(4)	C16—C17—N2—C21	-177.2(3)
C7—C8—C9—C10	175.4(5)	C18—C17—N2—Ru1	-164.1(3)
C13—C8—C9—C10	-0.8(7)	C16—C17—N2—Ru1	18.6(4)
C8—C9—C10—C11	-1.1(8)	C20—C21—N2—C17	0.3(6)
C9—C10—C11—C12	1.0(8)	C20—C21—N2—Ru1	162.7(3)
C10—C11—C12—C13	1.0(7)	N3—Ru1—N2—C17	-76.9(3)
C7—C8—C13—C14	3.5(6)	N1—Ru1—N2—C17	0.3(3)
C9—C8—C13—C14	179.8(4)	S1—Ru1—N2—C17	85.8(8)

C7—C8—C13—C12	-173.7(4)	Cl2—Ru1—N2—C17	-171.1(3)
C9—C8—C13—C12	2.6(6)	Cl1—Ru1—N2—C17	98.1(3)
C11—C12—C13—C14	-179.8(4)	N3—Ru1—N2—C21	120.2(3)
C11—C12—C13—C8	-2.7(6)	N1—Ru1—N2—C21	-162.6(3)
C2—C1—C14—C13	-173.2(4)	S1—Ru1—N2—C21	-77.1(8)
C6—C1—C14—C13	4.7(6)	Cl2—Ru1—N2—C21	26.0(3)
C2—C1—C14—C15	-0.9(6)	Cl1—Ru1—N2—C21	-64.8(3)
C6—C1—C14—C15	177.0(3)	C26—C27—N3—C23	1.5(6)
C8—C13—C14—C1	-5.8(6)	C26—C27—N3—Ru1	-178.1(3)
C12—C13—C14—C1	171.2(4)	C24—C23—N3—C27	-0.6(6)
C8—C13—C14—C15	-178.1(3)	C22—C23—N3—C27	-179.4(4)
C12—C13—C14—C15	-1.0(6)	C24—C23—N3—Ru1	179.0(3)
C1—C14—C15—N1	95.2(4)	C22—C23—N3—Ru1	0.2(4)
C13—C14—C15—N1	-92.5(4)	N2—Ru1—N3—C27	-81.2(4)
N1—C16—C17—N2	-35.2(5)	N1—Ru1—N3—C27	-160.7(4)
N1—C16—C17—C18	147.6(4)	S1—Ru1—N3—C27	100.9(3)
N2—C17—C18—C19	-0.1(7)	Cl2—Ru1—N3—C27	12.5(3)
C16—C17—C18—C19	176.9(4)	Cl1—Ru1—N3—C27	-150.2(8)
C17—C18—C19—C20	-0.2(7)	N2—Ru1—N3—C23	99.2(3)
C18—C19—C20—C21	0.5(8)	N1—Ru1—N3—C23	19.7(3)
C19—C20—C21—N2	-0.6(7)	S1—Ru1—N3—C23	-78.7(3)
N1—C22—C23—N3	-30.6(5)	Cl2—Ru1—N3—C23	-167.1(3)
N1—C22—C23—C24	150.6(4)	Cl1—Ru1—N3—C23	30.2(12)
N3—C23—C24—C25	-1.3(6)	N3—Ru1—S1—C28	-36.2(2)
C22—C23—C24—C25	177.4(4)	N2—Ru1—S1—C28	161.0(7)
C23—C24—C25—C26	2.3(7)	N1—Ru1—S1—C28	-114.6(2)
C24—C25—C26—C27	-1.5(7)	Cl2—Ru1—S1—C28	57.60(18)
C25—C26—C27—N3	-0.4(7)	Cl1—Ru1—S1—C28	148.80(18)
C23—C22—N1—C15	166.2(3)	N3—Ru1—S1—C29	-145.8(2)
C23—C22—N1—C16	-69.5(4)	N2—Ru1—S1—C29	51.4(8)
C23—C22—N1—Ru1	43.6(3)	N1—Ru1—S1—C29	135.9(2)
C14—C15—N1—C22	58.2(4)	Cl2—Ru1—S1—C29	-52.0(2)
C14—C15—N1—C16	-63.0(4)	Cl1—Ru1—S1—C29	39.2(2)
C14—C15—N1—Ru1	176.4(3)	N3—Ru1—S1—O1	89.39(18)
C17—C16—N1—C22	144.4(3)	N2—Ru1—S1—O1	-73.4(7)
C17—C16—N1—C15	-91.1(3)	N1—Ru1—S1—O1	11.02(17)
C17—C16—N1—Ru1	32.7(3)	Cl2—Ru1—S1—O1	-176.82(15)

Table S2. Selected bond lengths (Å) and angles (º) for Compound **3**

Pt1—N2	2.003 (3)	C26—C25	1.385 (5)
Pt1—N3	2.007 (3)	C26—C27	1.506 (5)
Pt1—N1	2.035 (3)	C15—H15A	0.9900
Pt1—Cl1	2.3065 (9)	C15—H15B	0.9900
N1—C21	1.506 (4)	C4—C5	1.337 (10)
N1—C27	1.506 (4)	C4—H4A	0.9500
N1—C15	1.527 (4)	C27—H27A	0.9900
N3—C16	1.340 (5)	C27—H27B	0.9900
N3—C20	1.354 (4)	C13—C8	1.415 (6)
N2—C26	1.343 (5)	C18—C17	1.370 (6)
N2—C22	1.355 (5)	C18—C19	1.381 (6)
C3—C2	1.365 (7)	C18—H18A	0.9500
C3—C4	1.404 (10)	C21—H21A	0.9900
C3—H3A	0.9500	C21—H21B	0.9900
C11—C12	1.346 (7)	C25—C24	1.366 (7)
C11—C10	1.394 (11)	C25—H25A	0.9500
C11—H11A	0.9500	C19—H19A	0.9500
C9—C10	1.363 (11)	C16—C17	1.375 (6)
C9—C8	1.440 (8)	C16—H16A	0.9500
C9—H9A	0.9500	C17—H17A	0.9500
C10—H10A	0.9500	C6—C7	1.388 (8)
C12—C13	1.447 (7)	C6—C5	1.429 (8)
C12—H12A	0.9500	C8—C7	1.399 (8)
C2—C1	1.426 (6)	C7—H7A	0.9500
C2—H2A	0.9500	C22—H22A	0.9500
C23—C22	1.366 (6)	C24—H24A	0.9500
C23—C24	1.385 (8)	C5—H5A	0.9500
C23—H23A	0.9500	P1—F1	1.501 (4)
C20—C19	1.377 (5)	P1—F6	1.549 (4)
C20—C21	1.508 (5)	P1—F2	1.564 (5)
C14—C13	1.412 (5)	P1—F4	1.569 (5)
C14—C1	1.417 (5)	P1—F5	1.580 (4)
C14—C15	1.498 (5)	P1—F3	1.574 (3)
C1—C6	1.438 (6)		

N2—Pt1—N3	167.04 (12)	N1—C27—H27A	109.7
N2—Pt1—N1	83.87 (12)	C26—C27—H27B	109.7
N3—Pt1—N1	84.48 (11)	N1—C27—H27B	109.7
N2—Pt1—Cl1	95.41 (9)	H27A—C27—H27B	108.2
N3—Pt1—Cl1	96.30 (9)	C8—C13—C14	120.1 (4)
N1—Pt1—Cl1	179.03 (8)	C8—C13—C12	115.9 (4)
C21—N1—C27	112.2 (3)	C14—C13—C12	124.0 (4)
C21—N1—C15	108.5 (3)	C17—C18—C19	119.2 (4)
C27—N1—C15	112.3 (3)	C17—C18—H18A	120.4
C21—N1—Pt1	105.4 (2)	C19—C18—H18A	120.4
C27—N1—Pt1	103.7 (2)	N1—C21—C20	110.7 (3)
C15—N1—Pt1	114.5 (2)	N1—C21—H21A	109.5
C16—N3—C20	118.9 (3)	C20—C21—H21A	109.5
C16—N3—Pt1	128.6 (2)	N1—C21—H21B	109.5
C20—N3—Pt1	112.5 (2)	C20—C21—H21B	109.5
C26—N2—C22	119.7 (3)	H21A—C21—H21B	108.1
C26—N2—Pt1	112.5 (2)	C24—C25—C26	119.1 (4)
C22—N2—Pt1	127.8 (3)	C24—C25—H25A	120.5
C2—C3—C4	121.0 (6)	C26—C25—H25A	120.5
C2—C3—H3A	119.5	C20—C19—C18	119.4 (4)
C4—C3—H3A	119.5	C20—C19—H19A	120.3
C12—C11—C10	120.3 (7)	C18—C19—H19A	120.3
C12—C11—H11A	119.9	N3—C16—C17	122.2 (4)
C10—C11—H11A	119.9	N3—C16—H16A	118.9
C10—C9—C8	119.3 (6)	C17—C16—H16A	118.9
C10—C9—H9A	120.4	C18—C17—C16	119.2 (4)
C8—C9—H9A	120.4	C18—C17—H17A	120.4
C9—C10—C11	121.3 (6)	C16—C17—H17A	120.4
C9—C10—H10A	119.4	C7—C6—C1	119.6 (5)
C11—C10—H10A	119.4	C7—C6—C5	122.4 (5)
C11—C12—C13	122.5 (6)	C1—C6—C5	118.0 (5)
C11—C12—H12A	118.7	C7—C8—C13	118.9 (4)
C13—C12—H12A	118.7	C7—C8—C9	120.5 (5)
C3—C2—C1	120.9 (5)	C13—C8—C9	120.6 (6)
C3—C2—H2A	119.5	C8—C7—C6	122.1 (4)
C1—C2—H2A	119.5	C8—C7—H7A	119.0

C22—C23—H23A	120.5	N2—C22—C23	121.3 (4)
C24—C23—H23A	120.5	N2—C22—H22A	119.3
N3—C20—C19	121.1 (3)	C23—C22—H22A	119.3
N3—C20—C21	116.1 (3)	C25—C24—C23	119.9 (4)
C19—C20—C21	122.5 (3)	C25—C24—H24A	120.0
C13—C14—C1	120.5 (4)	C23—C24—H24A	120.0
C13—C14—C15	119.6 (3)	C4—C5—C6	122.2 (5)
C1—C14—C15	119.9 (3)	C4—C5—H5A	118.9
C6—C1—C14	118.5 (4)	C6—C5—H5A	118.9
C6—C1—C2	117.9 (4)	F1—P1—F6	93.8 (4)
C14—C1—C2	123.6 (4)	F1—P1—F2	87.2 (5)
N2—C26—C25	121.0 (4)	F6—P1—F2	90.2 (3)
N2—C26—C27	115.5 (3)	F1—P1—F4	177.6 (4)
C25—C26—C27	123.3 (4)	F6—P1—F4	88.6 (4)
C14—C15—N1	114.6 (3)	F2—P1—F4	92.1 (4)
C14—C15—H15A	108.6	F1—P1—F5	94.1 (4)
N1—C15—H15A	108.6	F6—P1—F5	89.7 (3)
C14—C15—H15B	108.6	F2—P1—F5	178.7 (4)
N1—C15—H15B	108.6	F4—P1—F5	86.6 (3)
H15A—C15—H15B	107.6	F1—P1—F3	90.2 (3)
C5—C4—C3	120.0 (5)	F6—P1—F3	176.0 (3)
C5—C4—H4A	120.0	F2—P1—F3	89.4 (2)
C3—C4—H4A	120.0	F4—P1—F3	87.5 (3)
C26—C27—N1	109.9 (3)	F5—P1—F3	90.7 (2)
C26—C27—H27A	109.7		

N2—Pt1—N1—C21	−148.3 (2)	C25—C26—C27—N1	153.3 (3)
N3—Pt1—N1—C21	26.0 (2)	C21—N1—C27—C26	153.1 (3)
Cl1—Pt1—N1—C21	170 (5)	C15—N1—C27—C26	−84.4 (3)
N2—Pt1—N1—C27	−30.1 (2)	Pt1—N1—C27—C26	39.8 (3)
N3—Pt1—N1—C27	144.2 (2)	C1—C14—C13—C8	−6.2 (5)
Cl1—Pt1—N1—C27	−72 (5)	C15—C14—C13—C8	172.3 (3)
N2—Pt1—N1—C15	92.6 (2)	C1—C14—C13—C12	174.6 (4)
N3—Pt1—N1—C15	−93.1 (2)	C15—C14—C13—C12	−6.9 (5)
Cl1—Pt1—N1—C15	51 (5)	C11—C12—C13—C8	−3.1 (7)
N2—Pt1—N3—C16	−165.9 (4)	C11—C12—C13—C14	176.1 (5)

Cl1—Pt1—N3—C16	−11.3 (3)	C15—N1—C21—C20	88.3 (3)
N2—Pt1—N3—C20	13.3 (6)	Pt1—N1—C21—C20	−34.8 (3)
N1—Pt1—N3—C20	−12.7 (2)	N3—C20—C21—N1	27.6 (4)
Cl1—Pt1—N3—C20	167.9 (2)	C19—C20—C21—N1	−157.4 (3)
N3—Pt1—N2—C26	−10.6 (6)	N2—C26—C25—C24	−0.2 (6)
N1—Pt1—N2—C26	15.5 (2)	C27—C26—C25—C24	175.2 (4)
Cl1—Pt1—N2—C26	−165.2 (2)	N3—C20—C19—C18	1.6 (6)
N3—Pt1—N2—C22	170.8 (4)	C21—C20—C19—C18	−173.1 (4)
N1—Pt1—N2—C22	−163.1 (3)	C17—C18—C19—C20	−1.1 (7)
Cl1—Pt1—N2—C22	16.3 (3)	C20—N3—C16—C17	−0.6 (5)
C8—C9—C10—C11	−2.5 (11)	Pt1—N3—C16—C17	178.5 (3)
C12—C11—C10—C9	3.8 (11)	C19—C18—C17—C16	−0.2 (7)
C10—C11—C12—C13	−0.9 (9)	N3—C16—C17—C18	1.0 (6)
C4—C3—C2—C1	0.3 (7)	C14—C1—C6—C7	−0.2 (6)
C16—N3—C20—C19	−0.7 (5)	C2—C1—C6—C7	179.6 (4)
Pt1—N3—C20—C19	−180.0 (3)	C14—C1—C6—C5	−179.8 (4)
C16—N3—C20—C21	174.3 (3)	C2—C1—C6—C5	0.0 (6)
Pt1—N3—C20—C21	−5.0 (4)	C14—C13—C8—C7	3.8 (6)
C13—C14—C1—C6	4.3 (5)	C12—C13—C8—C7	−176.9 (4)
C15—C14—C1—C6	−174.1 (3)	C14—C13—C8—C9	−174.9 (4)
C13—C14—C1—C2	−175.4 (4)	C12—C13—C8—C9	4.4 (6)
C15—C14—C1—C2	6.1 (5)	C10—C9—C8—C7	179.5 (6)
C3—C2—C1—C6	0.5 (6)	C10—C9—C8—C13	−1.7 (9)
C3—C2—C1—C14	−179.7 (4)	C13—C8—C7—C6	0.3 (7)
C22—N2—C26—C25	−0.9 (5)	C9—C8—C7—C6	179.1 (5)
Pt1—N2—C26—C25	−179.6 (3)	C1—C6—C7—C8	−2.1 (7)
C22—N2—C26—C27	−176.7 (3)	C5—C6—C7—C8	177.4 (4)
Pt1—N2—C26—C27	4.6 (4)	C26—N2—C22—C23	0.8 (6)
C13—C14—C15—N1	−90.2 (4)	Pt1—N2—C22—C23	179.3 (3)
C1—C14—C15—N1	88.3 (4)	C24—C23—C22—N2	0.5 (8)
C21—N1—C15—C14	171.8 (3)	C26—C25—C24—C23	1.5 (7)
C27—N1—C15—C14	47.2 (4)	C22—C23—C24—C25	−1.6 (8)
Pt1—N1—C15—C14	−70.8 (3)	C3—C4—C5—C6	2.3 (8)
C2—C3—C4—C5	−1.7 (8)	C7—C6—C5—C4	179.0 (5)

Table S5. Bond lengths (Å) and angles (º) of hydrogen bonds for Compound **1**

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C(20)-H(20A) ..Cl(1)	0.93	2.80	3.545(5)	137
Intra C(21)-H(21A) ..Cl(2)	0.93	2.72	3.291(5)	121
C(26)-H(26A) ..Cl(2)	0.93	2.76	3.328(5)	120
Intra C(27)-H(27A) ..Cl(1)	0.93	2.81	3.620(5)	147

Symmetry codes: (i) 1/2-x,1/2+y,1/2+z; (ii) 1/2-x,-1/2+y,1/2+z

Table S7. Bond lengths (Å) and angles (º) of hydrogen bonds for Compound **2**

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
Intra C(15)-H(15A) ..Cl(1)	0.95	2.62	3.27(4)	125
C(20)-H(20A) ..Cl(1)	0.95	2.79	3.64(5)	149
Intra C(21)-H(21A) ..Cl(2)	0.94	2.74	3.36(5)	123
C(22)-H(22A) ..Cl(2)	0.98	2.65	3.56(6)	155
Intra C(27)-H(27A) ..Cl(2)	0.96	2.73	3.34(6)	122
Intra C(29)-H(29C) ..Cl(1)	0.99	2.71	3.30(7)	118

Symmetry codes: (i) 2/3-x,1/3-y,1/3-z; (ii) x-y,x,-z

Table S6. Bond lengths (Å) and angles (º) of hydrogen bonds for Compound **3**

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C(15)-H(15A) ..F(3)	0.99	2.50	3.2461	132
C(15)-H(15A) ..F(5)	0.99	2.52	3.4874	165
Intra C(16)-H(16A) ..Cl(1)	0.95	2.79	3.3512	118
C(19)-H(19A) ..Cl(1)	0.95	2.72	3.5292	143
C(21)-H(21B) ..Cl(1)	0.99	2.79	3.7378	161
Intra C(22)-H(22A) ..Cl(1)	0.95	2.77	3.3177	118
C(23)-H(23A) ..F(6)	0.95	2.54	3.3353	142
C(25)-H(25A) ..F(4)	0.95	2.55	3.4044	151
C(27)-H(27B) ..Cl(1)	0.99	2.65	3.5904	159

Symmetry codes: (i) -x,-y,2-z; (ii) 1+x,y,z; (iii) 1-x,-y,1-z; (v) -x,1-y,1-z; (iv)1-x,1-y,1-z