Electronic Supplementary Material (ESI)

Isoelectronic Pt(II)- and Au(III)-*N*-Heterocyclic Carbene Complexes: A Structural and Biological Comparison

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Table S1. Summary of crystallographic data recorded for complexes **2** and **3**.

	2	**3**
Empirical formula	$[C_{26}H_{22}ClN_6Pt \bullet PF_6 \bullet ½(C_2H_3N)]$	$[C_{26}H_{22}AuClF_{12}N_6P_2]$
Formula weight	814.53	940.85
Crystal system	Monoclinic	Monoclinic
Space group	C2/c	$P2_1/c$
Temperature (K)	295	150(2)
Wavelength	0.71073	0.71073
Cell dimensions		
a (Å)	31.6422(2)	8.5767(12)
b (Å)	9.3109(1)	14.938(2)
c (Å)	24.2935(2)	24.059(3)
α (°) = γ(°)	90.00	90.00
β (°)	126.6131(6)	97.704(3)
Volume ($Å^3$)	5745.02(9)	3054.5(7)
Z	8	4
Density (g cm^{-3})	1.883	2.046
Absorption coefficient (mm^{-1})	5.103	5.113
Theta range for data collection	$2\vartheta < 60°$	$2\vartheta < 55°$
Observed data/no. of parameter	6685/387	5412/435
Tot. data/Uniq. data/R (int)	32352/8314/0.0466	28037/5380/0.0489
Final R indices [I > 2σ(I)]	R1 = 0.0419, wR2 = 0.0986	R1 = 0.0318, wR2 = 0.0776
Goodness-of-fit on F2	1.046	1.048

Table S2. Energies and compositions of selected molecular orbitals calculated for **2** and **3**.

MO	Energy (eV)	% composition		
Complex **2**		Pt	L	Cl
LUMO+5	-3.10	06	93	01
LUMO+4	-3.45	03	96	0
LUMO+3	-3.60	07	93	0
LUMO+2	-3.85	01	99	0
LUMO+1	-4.21	02	98	0
LUMO	-4.94	06	93	01
HOMO	-8.01	05	94	01
HOMO-1	-8.28	18	71	11
HOMO-2	-9.22	29	12	59
HOMO-3	-9.28	22	24	54
HOMO-4	-9.37	55	20	24
HOMO-5	-9.83	20	79	01
HOMO-6	-9.98	47	50	03
HOMO-7	-10.06	01	98	01
HOMO-8	-10.15	28	72	01
HOMO-9	-10.28	05	92	02
HOMO-10	-10.54	02	92	06
Complex **3**		Au	L	Cl
LUMO+5	-6.32	06	94	0
LUMO+4	-6.71	09	90	01
LUMO+3	-7.05	01	99	0
LUMO+2	-7.31	01	99	0
LUMO+1	-8.26	07	93	0
LUMO	-8.47	35	48	17
HOMO	-11.27	01	98	01
HOMO-1	-11.69	03	96	01
HOMO-2	-12.54	0	99	01
HOMO-3	-13.04	04	88	09
HOMO-4	-13.16	03	71	26
HOMO-5	-13.22	03	43	53
HOMO-6	-13.32	03	59	37
HOMO-7	-13.34	05	49	46
HOMO-8	-13.46	01	93	05
HOMO-9	-14.14	0	99	01
HOMO-10	-14.20	02	93	05

Table S3. Selected vertical electronic excitations calculated for complex **2**.

$E_{excitation}$ (eV)	$\lambda_{excitation}$ (nm)	Osc. Strength (f)	Key transitions	Character
2.1917	565.7	0.0078	(98%) HOMO→LUMO	L(π)→Au(dπ)/L(π^*)
3.0056	412.5	0.0943	(99%) HOMO-1→LUMO+1	L(π)→L(π^*)
3.6987	335.2	0.1313	(93%) HOMO→LUMO+2	L(π)→L(π^*)
4.4620	277.9	0.2290	(64%) HOMO-1→LUMO+4	L(π)→L(π^*)
4.4866	276.3	0.1289	(82%) HOMO→LUMO+6	L(π)→L(π^*)
4.9279	251.6	0.1789	(65%) HOMO-6→LUMO+1	L(π)/Cl(π)→L(π^*)
5.0385	246.1	0.2435	(37%) HOMO-4→LUMO+2	L(π)/Cl(π)→L(π^*)
			(26%) HOMO-2→LUMO+2	L(π)→ L(π^*)
5.0614	244.9	0.3126	(35%) HOMO-2→LUMO+2	L(π)→ L(π^*)
			(32%) HOMO-4→LUMO+2	L(π)/Cl(π)→L(π^*)

Table S4. Selected vertical electronic excitations calculated for **3**.

$E_{excitation}$ (eV)	$\lambda_{excitation}$ (nm)	Osc. Strength (f)	Key transitions	Character
2.8382	436.9	0.0127	(84%) HOMO→LUMO	L(π)→L(π^*)
2.8479	435.3	0.0787	(83%) HOMO-1→LUMO	L(π)→L(π^*)
3.5677	347.5	0.0423	(93%) HOMO-1→LUMO+1	L(π)→L(π^*)
3.6017	344.2	0.0935	(77%) HOMO→LUMO+2	L(π)→L(π^*)
4.3917	282.3	0.0405	(59%) HOMO-5→LUMO	L(π)→L(π^*)
4.4620	277.8	0.0477	(39%) HOMO-2→LUMO+2 (33%) HOMO-2→LUMO+4	Pt(dπ)/Cl(π)→ L(π^*)
4.5325	273.5	0.0827	(33%) HOMO-2→LUMO+2 (30%) HOMO-6→LUMO	Pt(dπ)/Cl(π)→ L(π^*)
4.7577	260.6	0.3636	(44%) HOMO-1→LUMO+7 (24%) HOMO→LUMO+8	L(π)→ L(π^*)
4.8379	256.3	0.2464	(57%) HOMO→LUMO+8	L(π)→L(π^*)
5.2033	238.3	0.1622	(59%) HOMO-5→LUMO+1	L(π)→L(π^*)

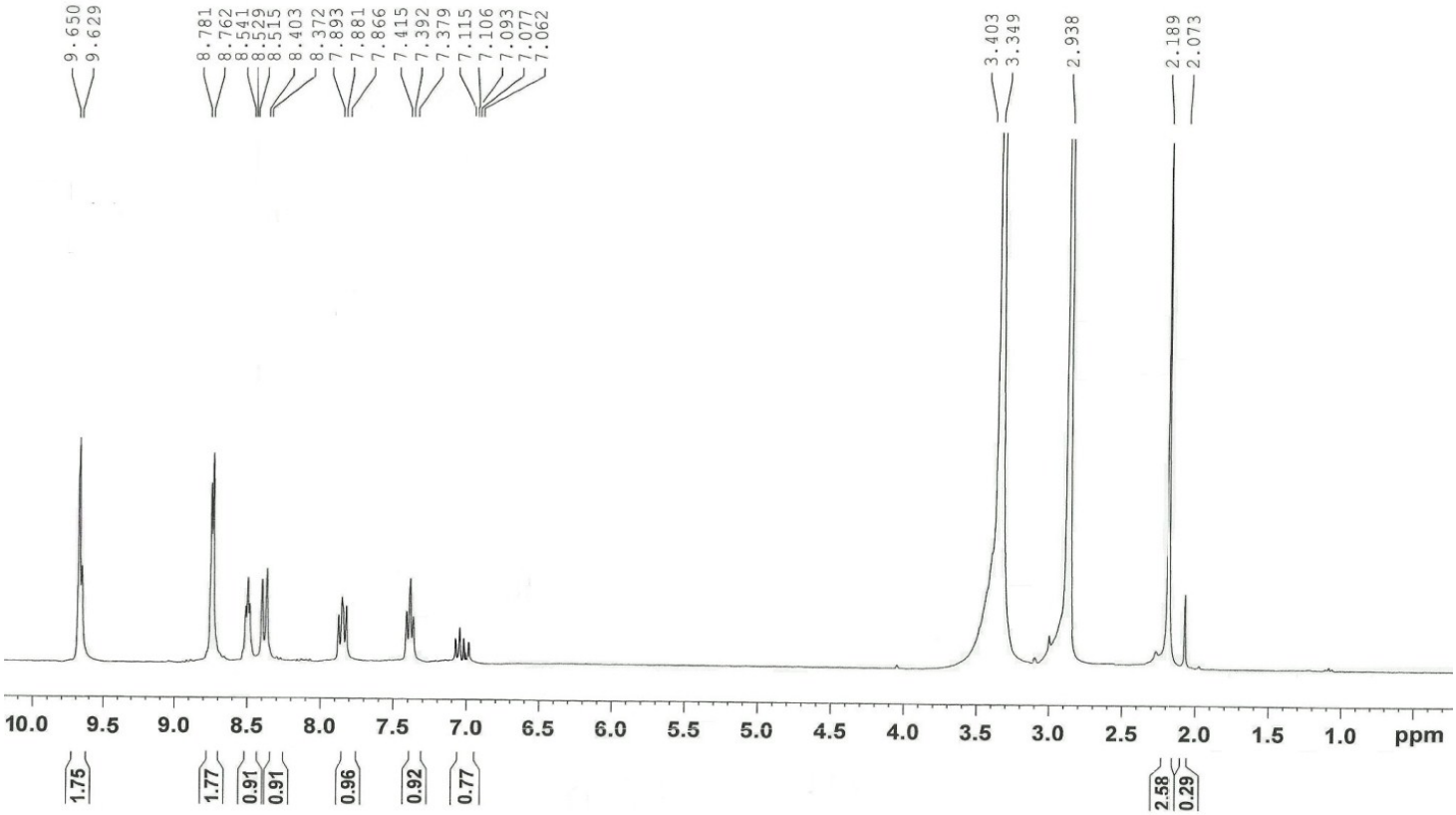

Figure S1. ^{1}H NMR spectrum of **2**.

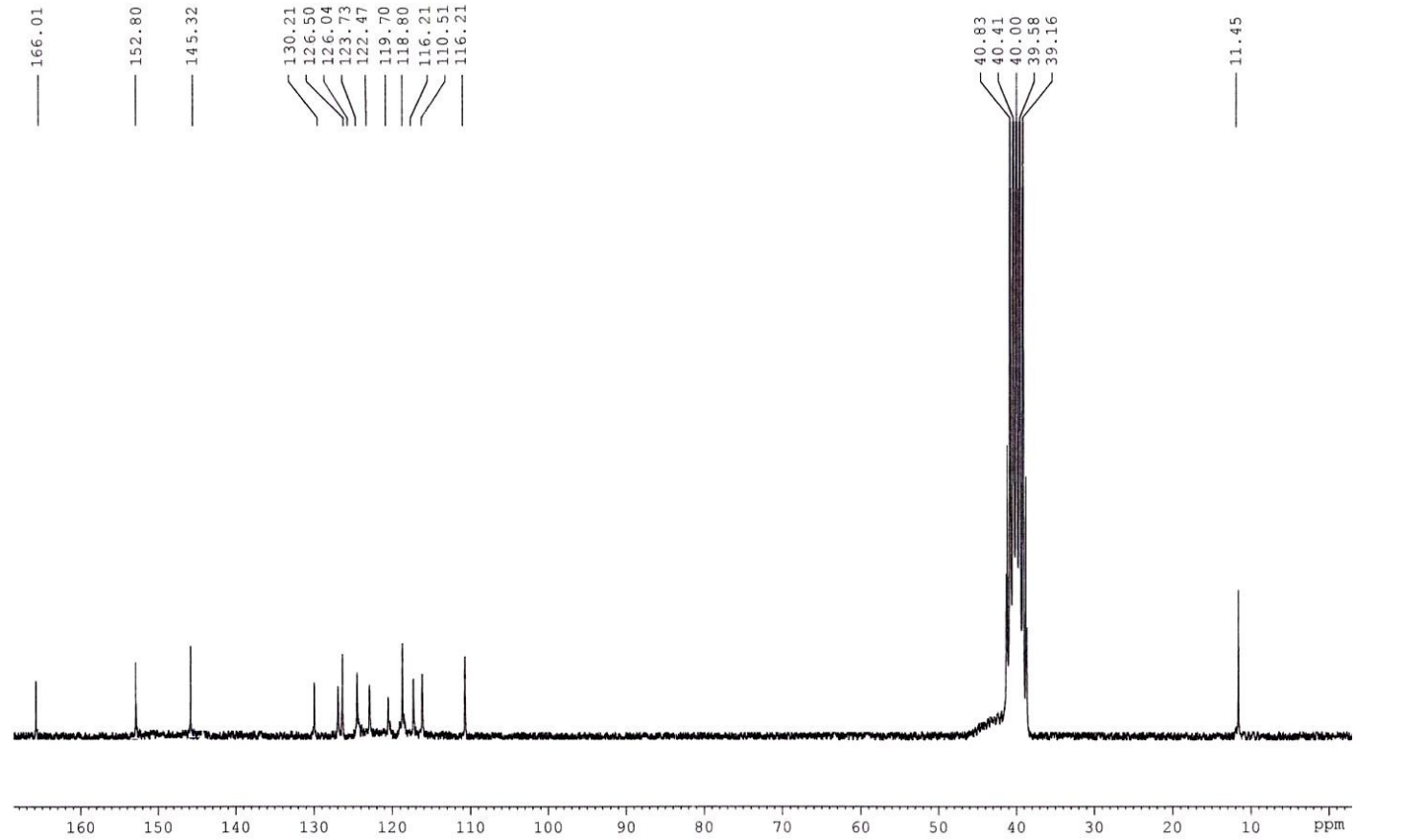

Figure S2. ^{13}C NMR spectrum of **2**.

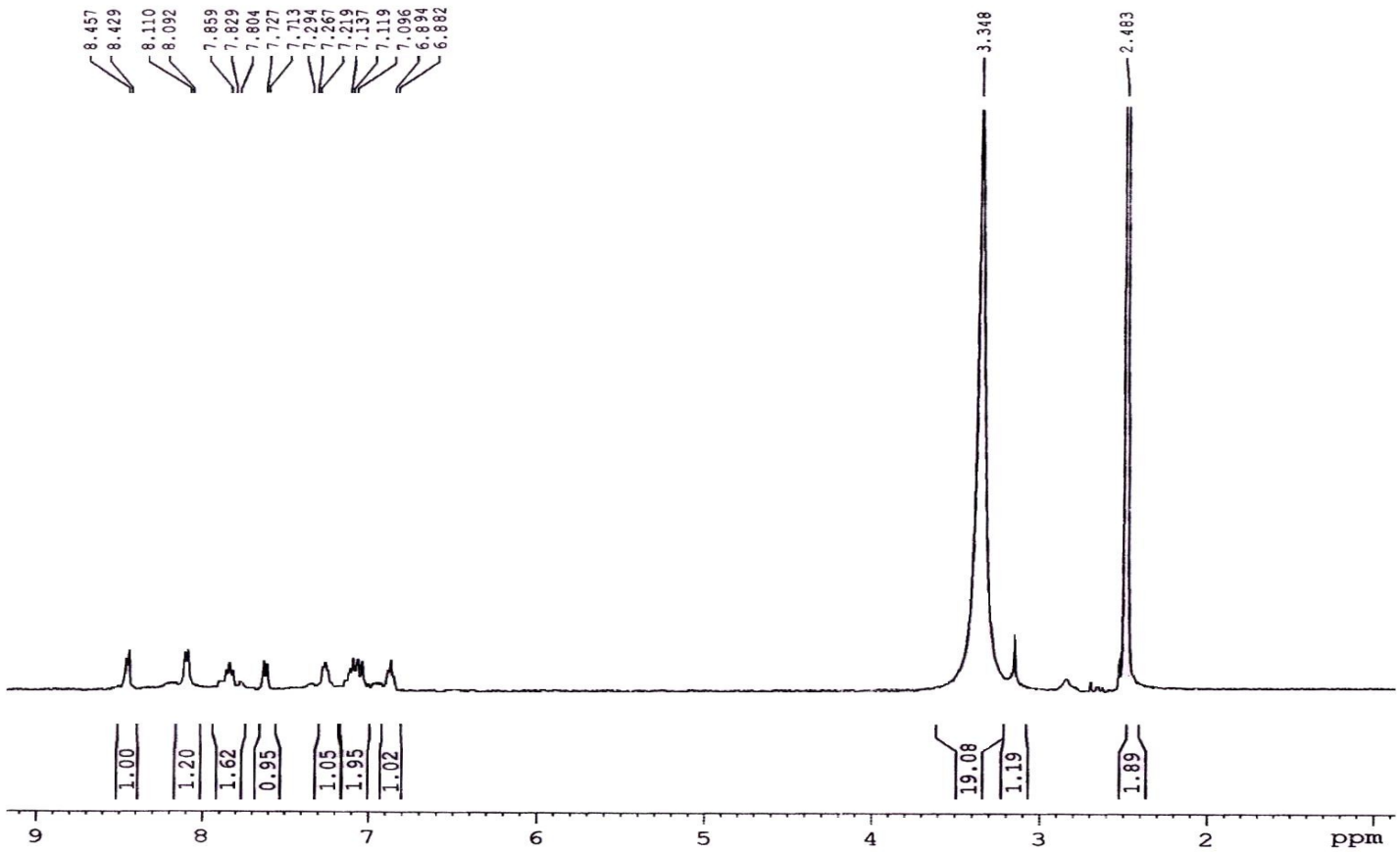

Figure S3. ^{1}H NMR spectrum of **3**.

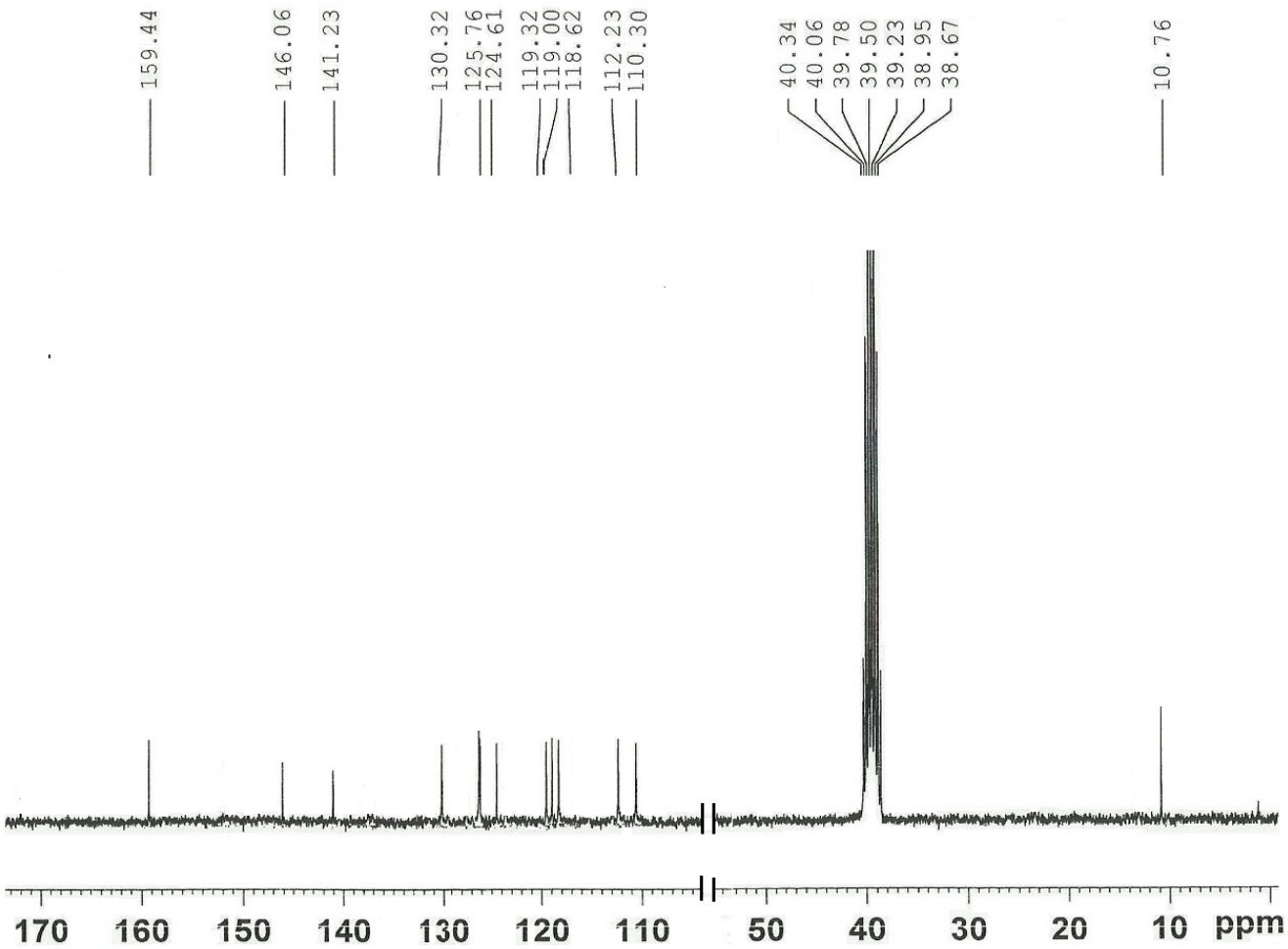

Figure S4. ^{13}C NMR spectrum of **3**.

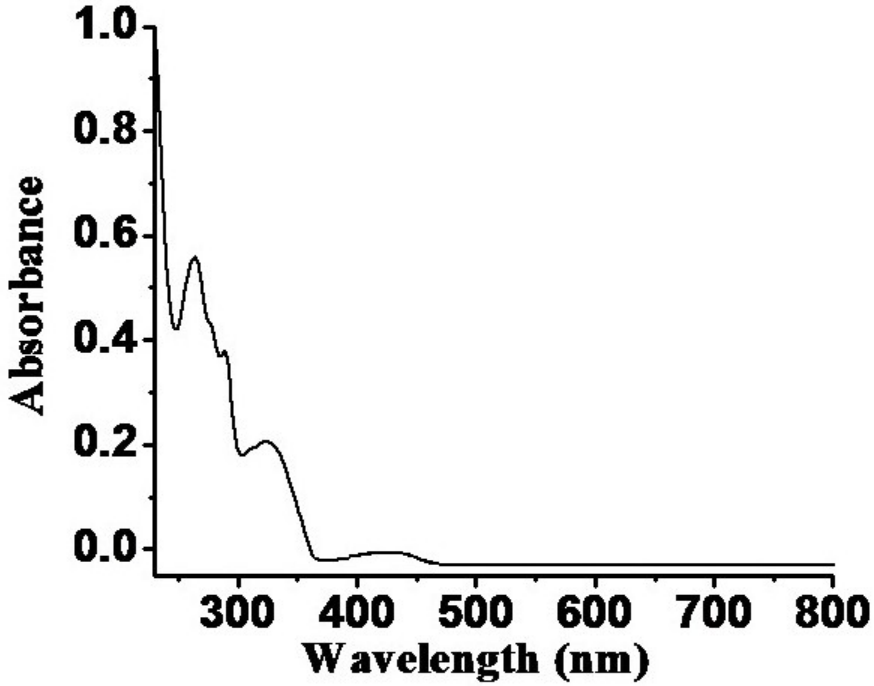

Figure S5. UV-vis spectrum of complex **2**.