Electronic Supplementary Information

Photophysical Properties of a Series of Cycloplatinated(II) Complexes Featuring Allyldiphenylphosphane

Hamid R. Shahsavari,[a]* Reza Babadi Aghakhanpour,[a,c] Mojgan Babaghasabha,[a] Mohsen Golbon Haghighi,[b] S. Masoud Nabavizadeh[c] and Behrouz Notash[b]

[a]*Department of Chemistry, Institute for Advanced Studies in Basic Sciences (IASBS), Yousef Sobouti Blvd., Zanjan 45137-6731, Iran.*

[b]*Department of Chemistry, Shahid Beheshti University, Evin, Tehran 19839-69411, Iran.*

[c]*Department of Chemistry, College of Sciences, Shiraz University, Shiraz, 71454, Iran.*

Email: shahsavari@iasbs.ac.ir

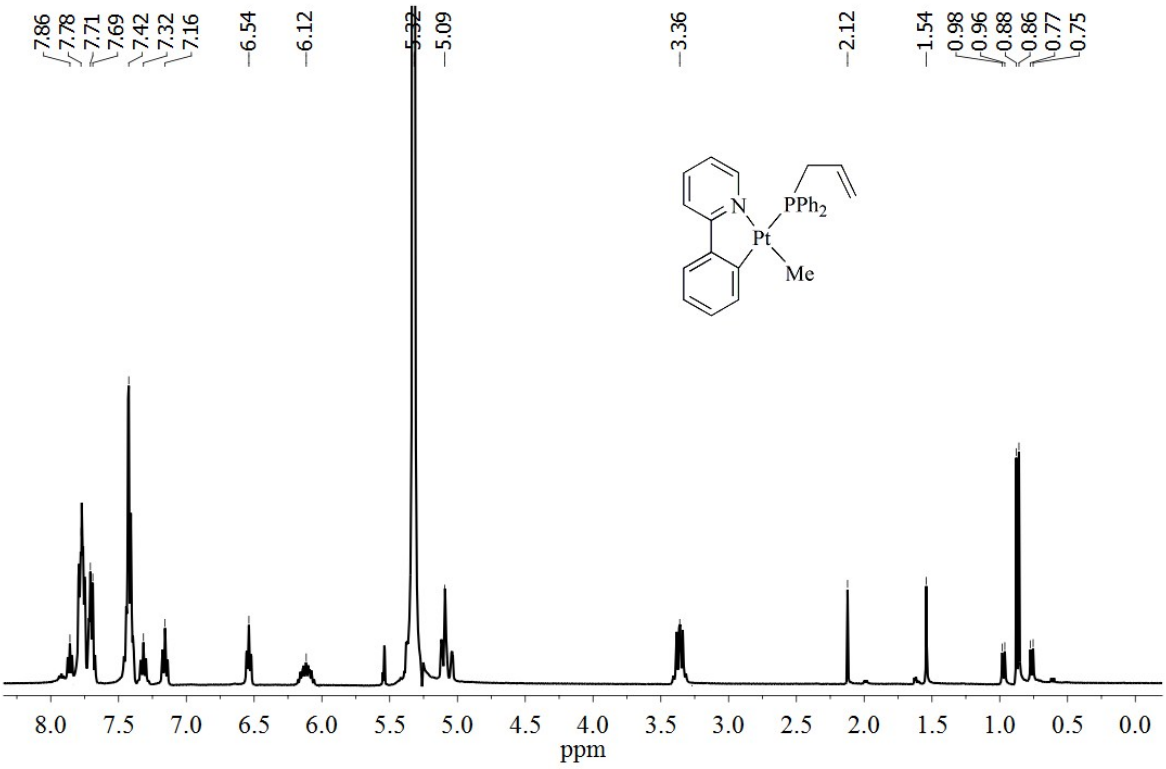


Figure S1. ^{1}HNMR spectrum of [Pt(ppy)(Me)(PPh_2allyl)], **1**, in CD_2Cl_2.

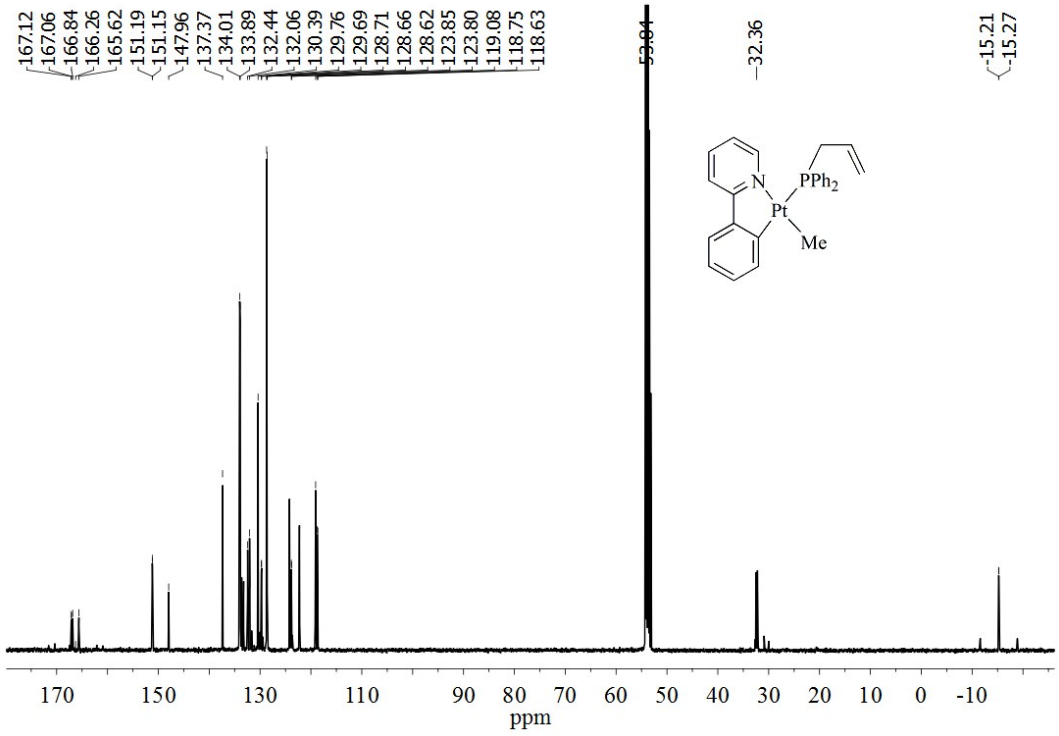


Figure S2. ^{13}CNMR spectrum of [Pt(ppy)(Me)(PPh_2allyl)], **1**, in CD_2Cl_2.

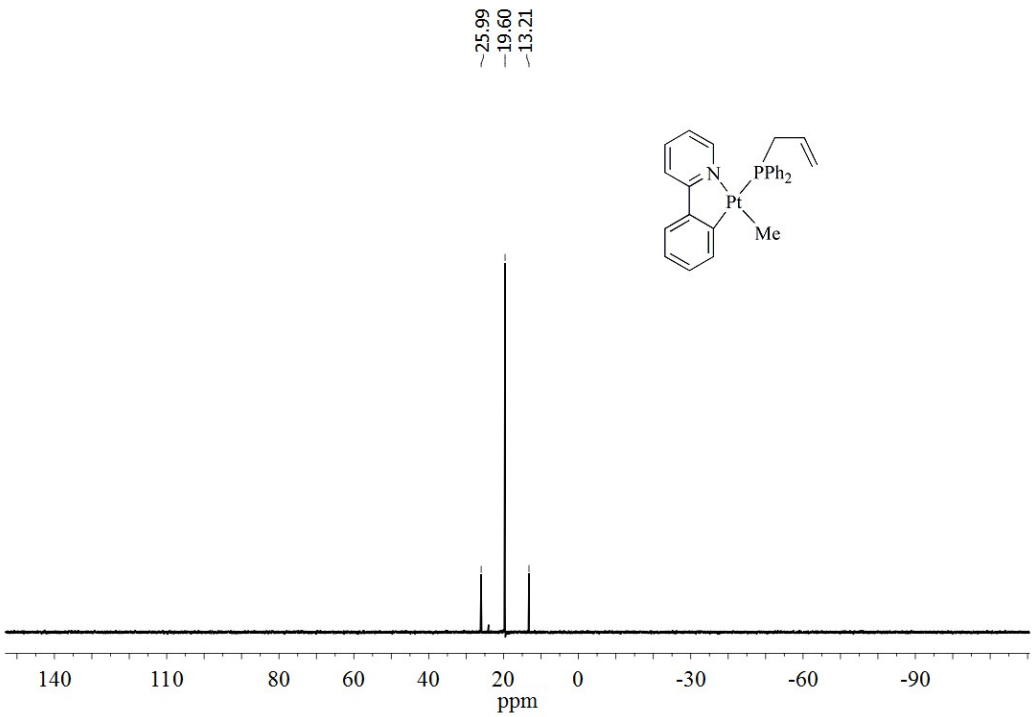


Figure S3. ^{31}PNMR spectrum of [Pt(ppy)(Me)(PPh_2allyl)],**1**, in CD_2Cl_2.

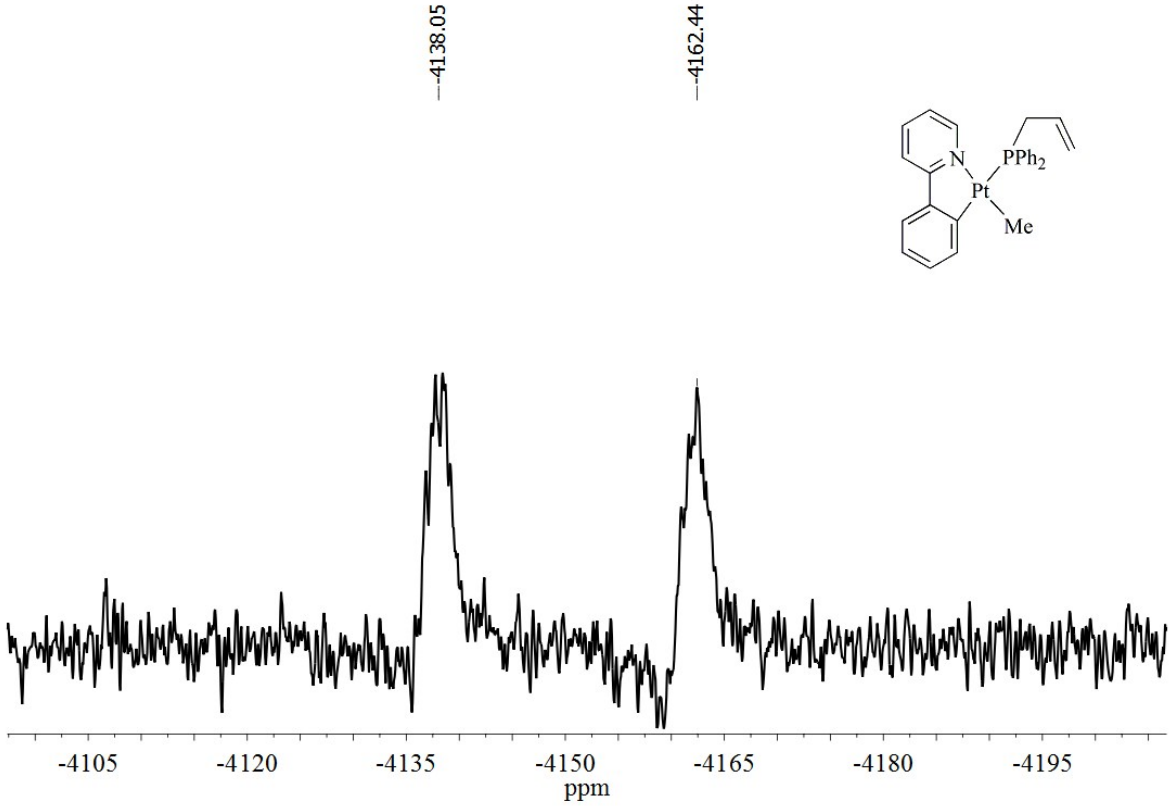


Figure S4. ^{195}PtNMR spectrum of [Pt(ppy)(Me)(PPh_2allyl)], **1**, in CD_2Cl_2.

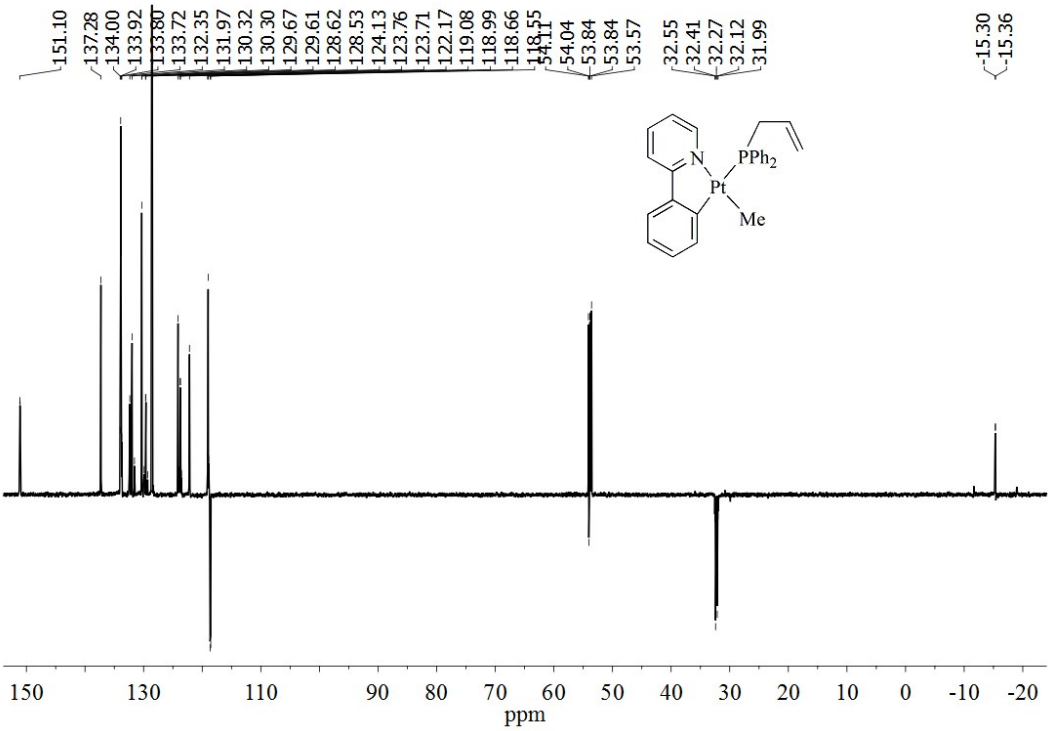


Figure S5. DEPT 135° spectrum of [Pt(ppy)(Me)(PPh_2allyl)], **1**, in CD_2Cl_2.

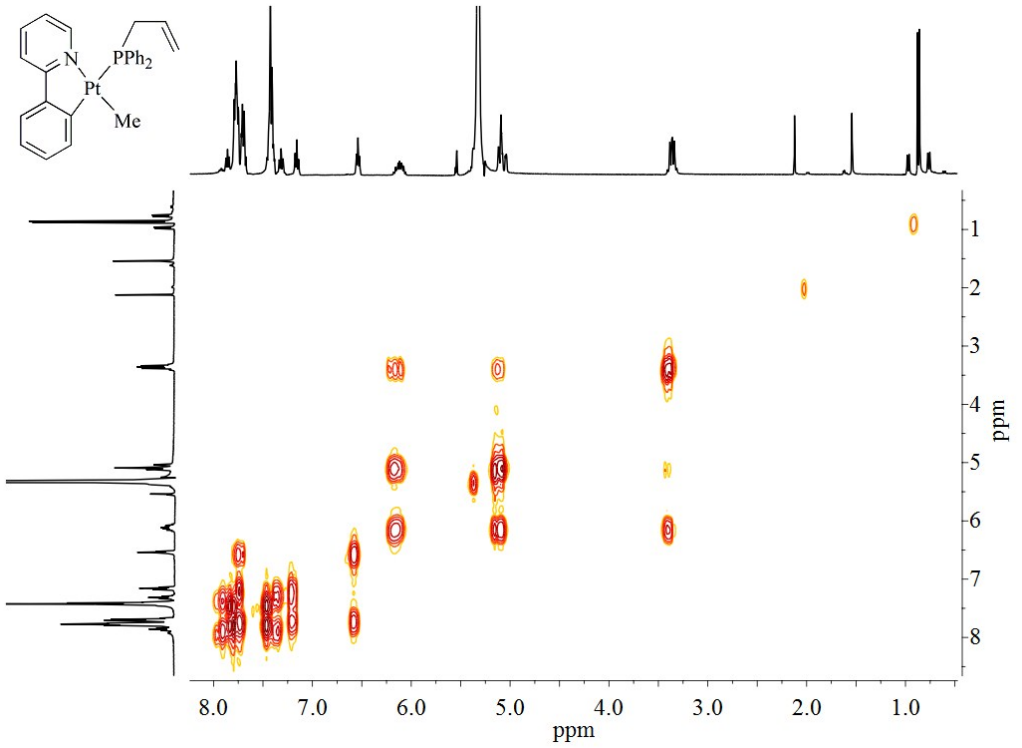


Figure S6. HHCOSY spectrum of [Pt(ppy)(Me)(PPh_2allyl)], **1**, in CD_2Cl_2.

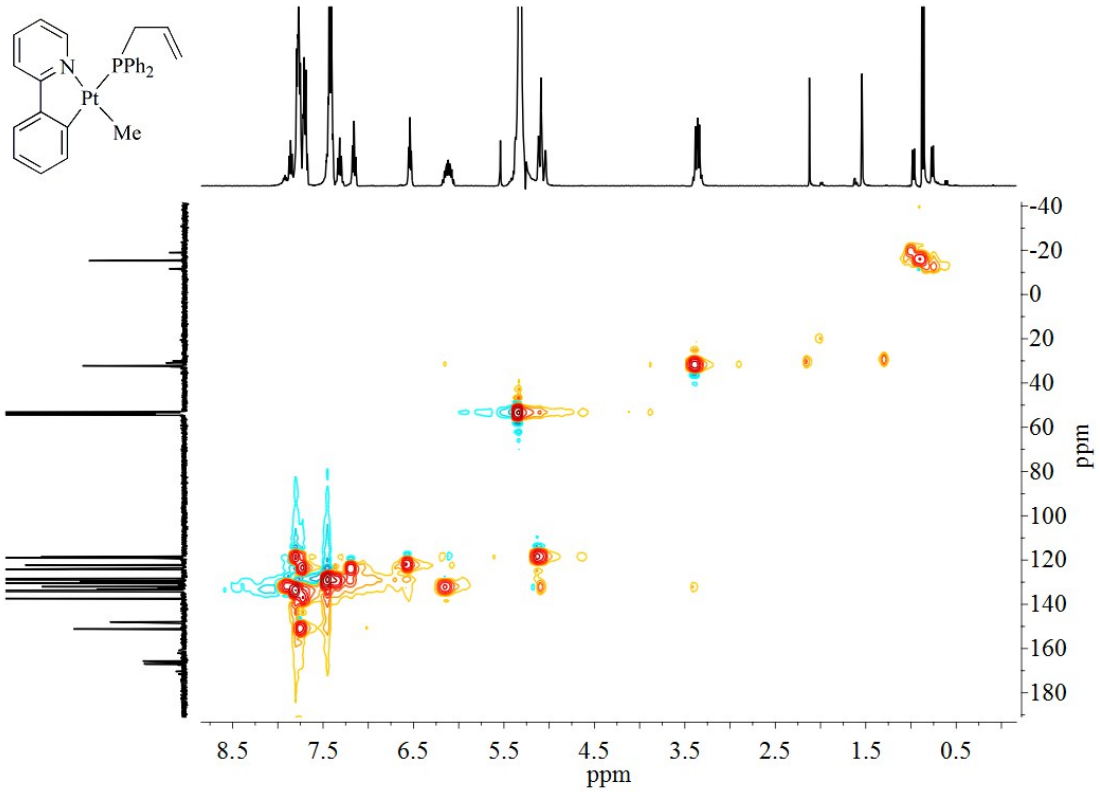


Figure S7. HSQC spectrum of [Pt(ppy)(Me)(PPh_2allyl)], **1**, in CD_2Cl_2.

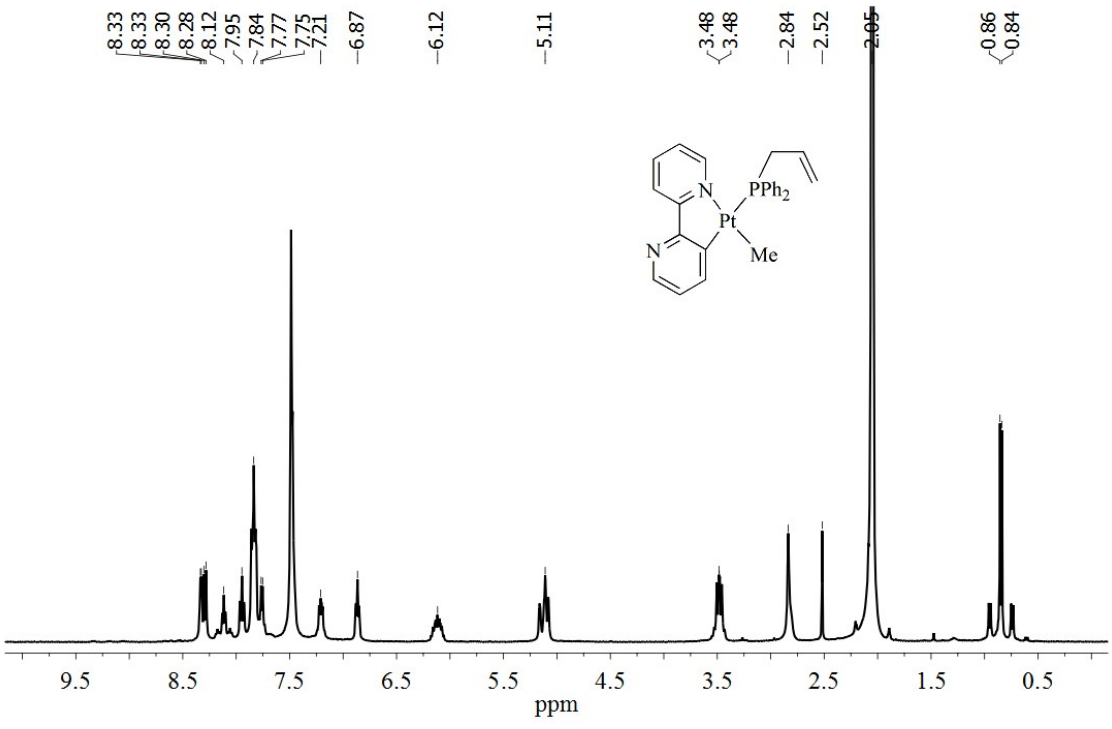


Figure S8.[1]HNMR spectrum of [Pt(bpy)(Me)(PPh_2allyl)], **2**, in acetone-d_6.

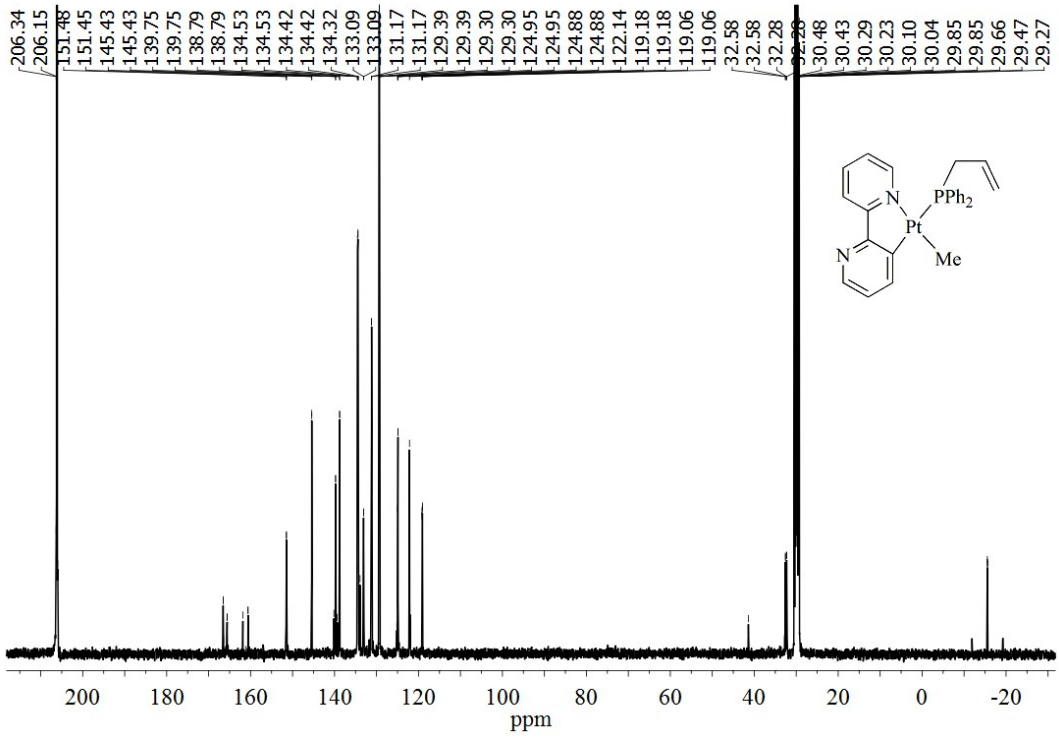


Figure S9. ^{13}CNMR spectrum of [Pt(bpy)(Me)(PPh$_2$allyl)], **2**, in acetone-d_6.

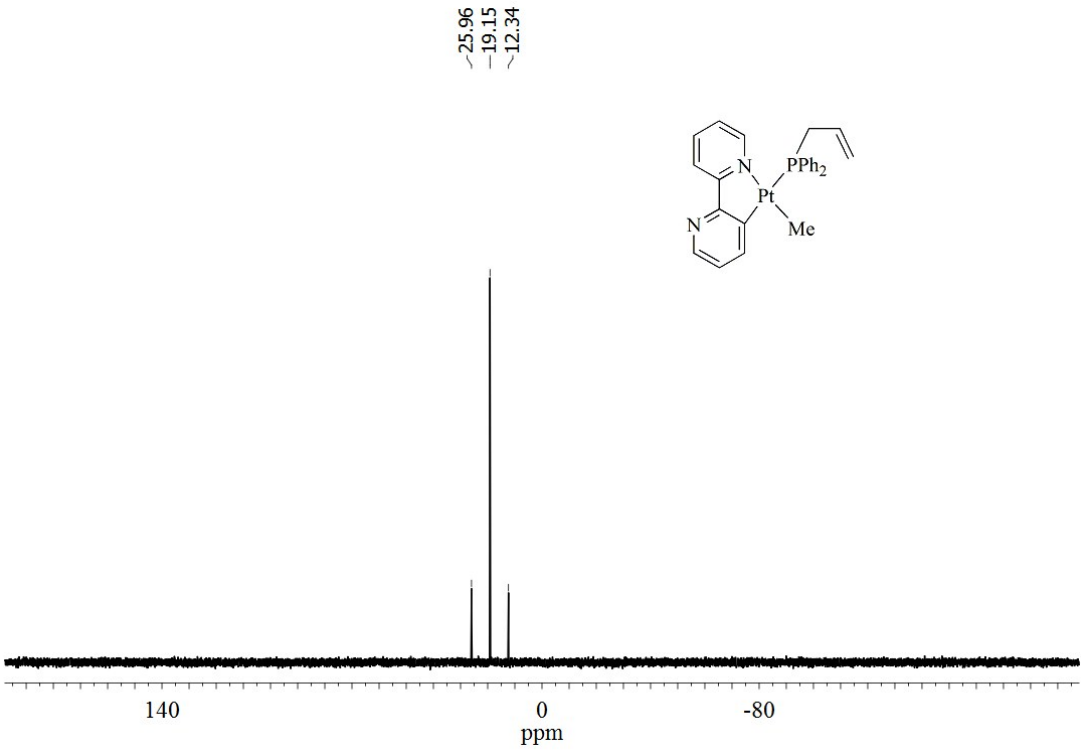


Figure S10. ^{31}PNMR spectrum of [Pt(bpy)(Me)(PPh$_2$allyl)], **2**, in acetone-d_6.

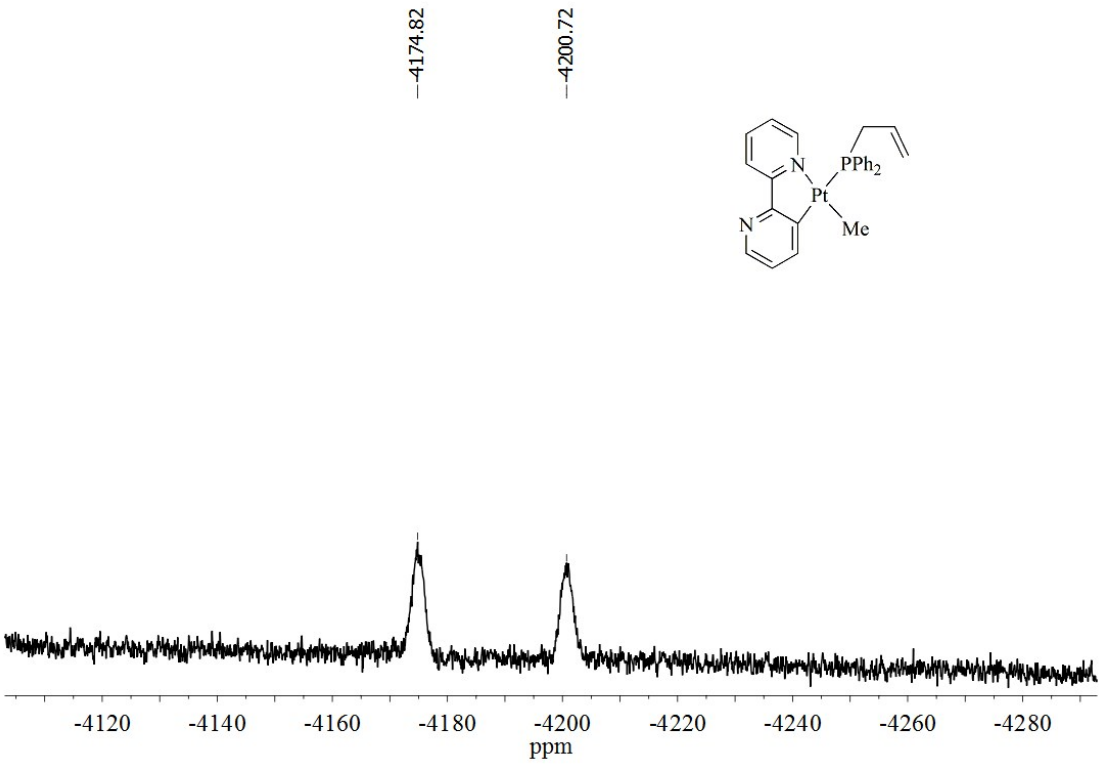


Figure S11. ^{195}PtNMR spectrum of [Pt(bpy)(Me)(PPh$_2$allyl)], **2**, in acetone-d_6.

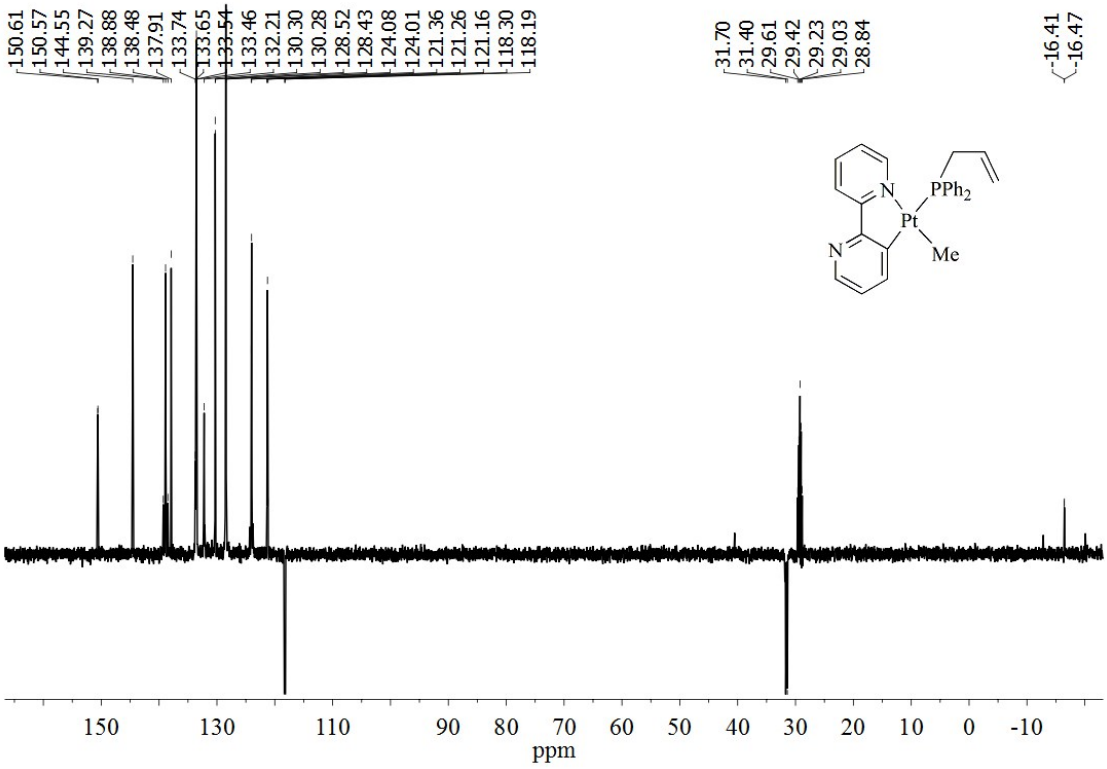


Figure S12. DEPT 135° spectrum of [Pt(bpy)(Me)(PPh$_2$allyl)], **2**, in acetone-d_6.

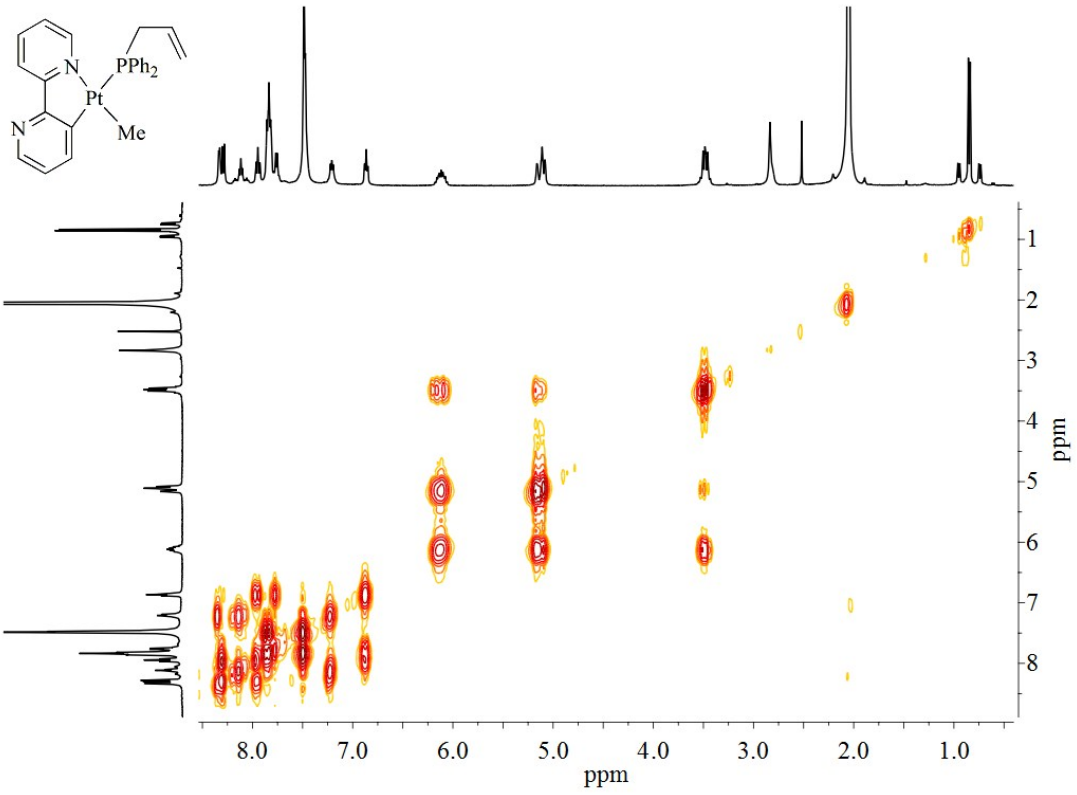


Figure S13. HHCOSY spectrum of [Pt(bpy)(Me)(PPh_2allyl)], **2**,in acetone-d_6.

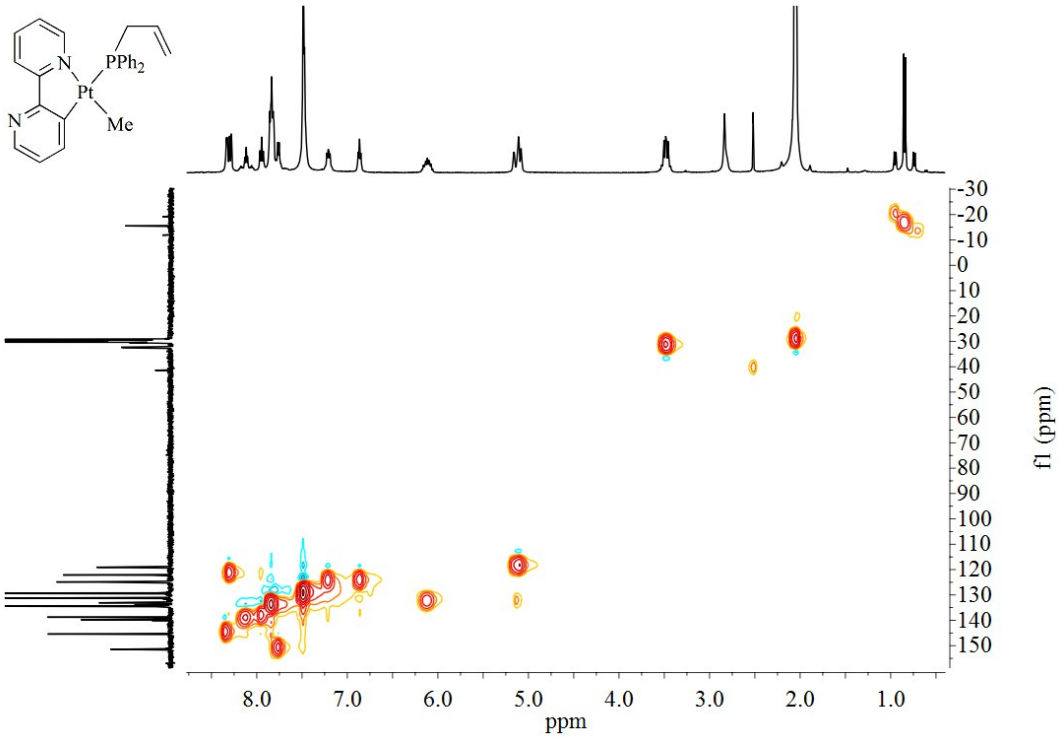


Figure S14. HSQC spectrum of [Pt(bpy)(Me)(PPh_2allyl)], **2**, in acetone-d_6**.**

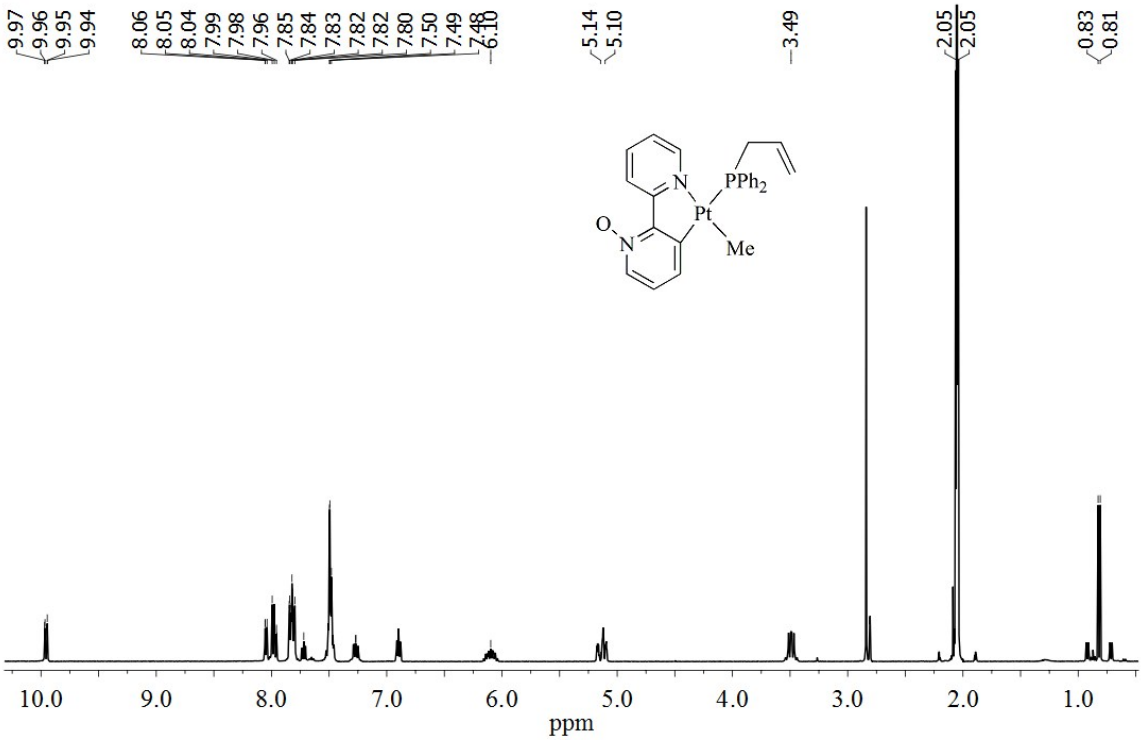


Figure S15. [1]HNMR spectrum of [Pt(O-bpy)(Me)(PPh_2allyl)], **3**, in acetone-d_6.

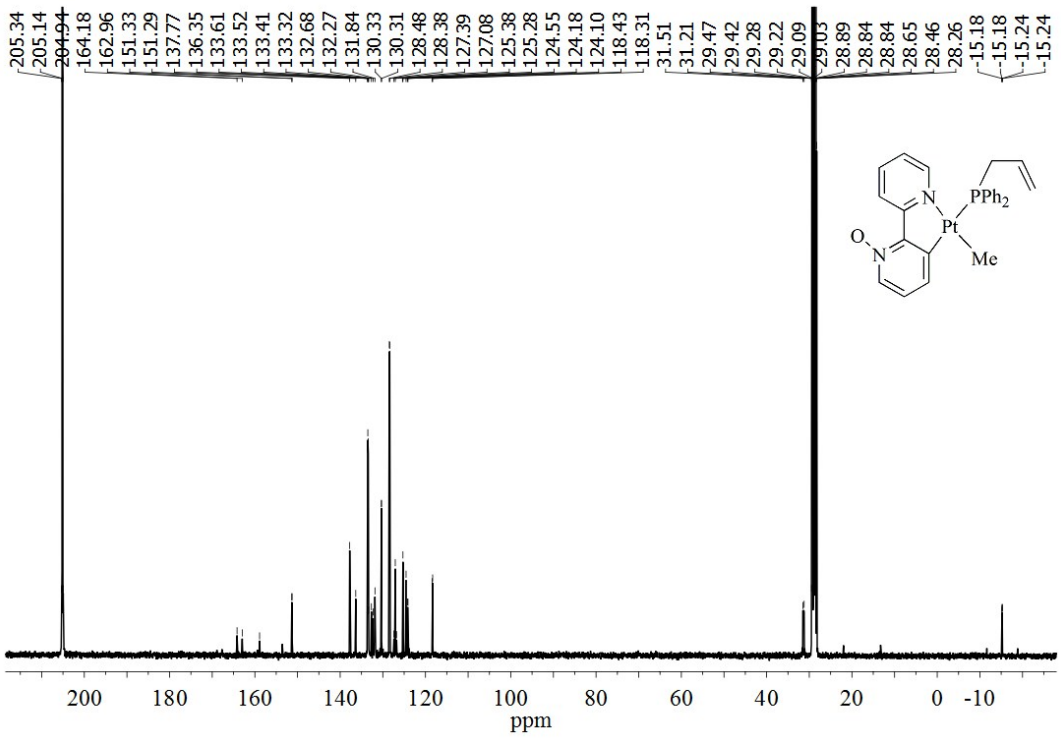


Figure S16. [13]CNMR spectrum of [Pt(O-bpy)(Me)(PPh_2allyl)], **3**, in acetone-d_6.

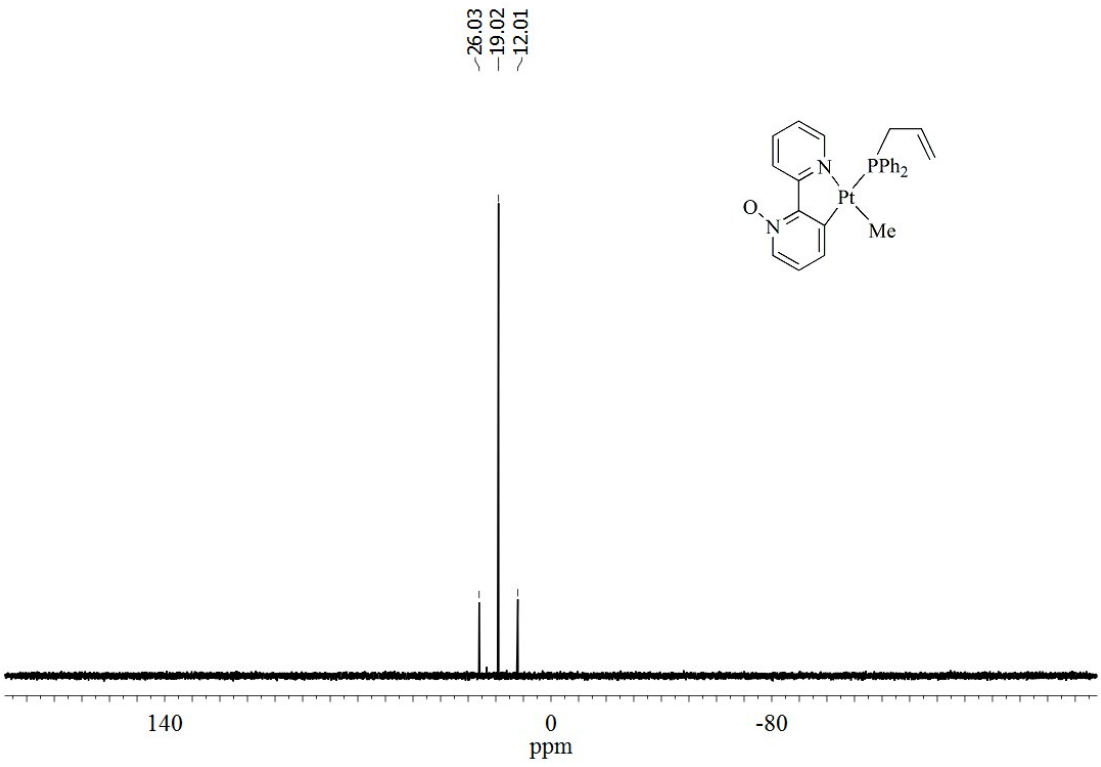


Figure S17. ^{31}PNMR spectrum of [Pt(O-bpy)(Me)(PPh_2allyl)], **3**, in acetone-d_6.

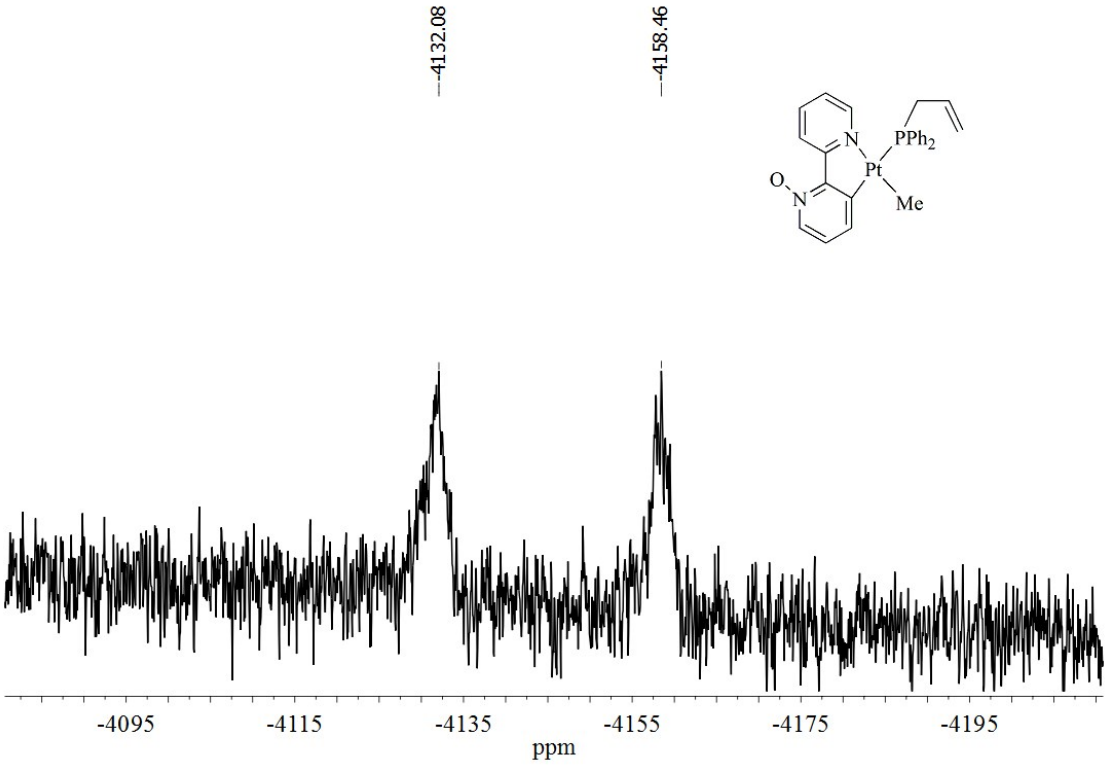


Figure S18. ^{195}PtNMR spectrum of [Pt(O-bpy)(Me)(PPh_2allyl)], **3**, in acetone-d_6.

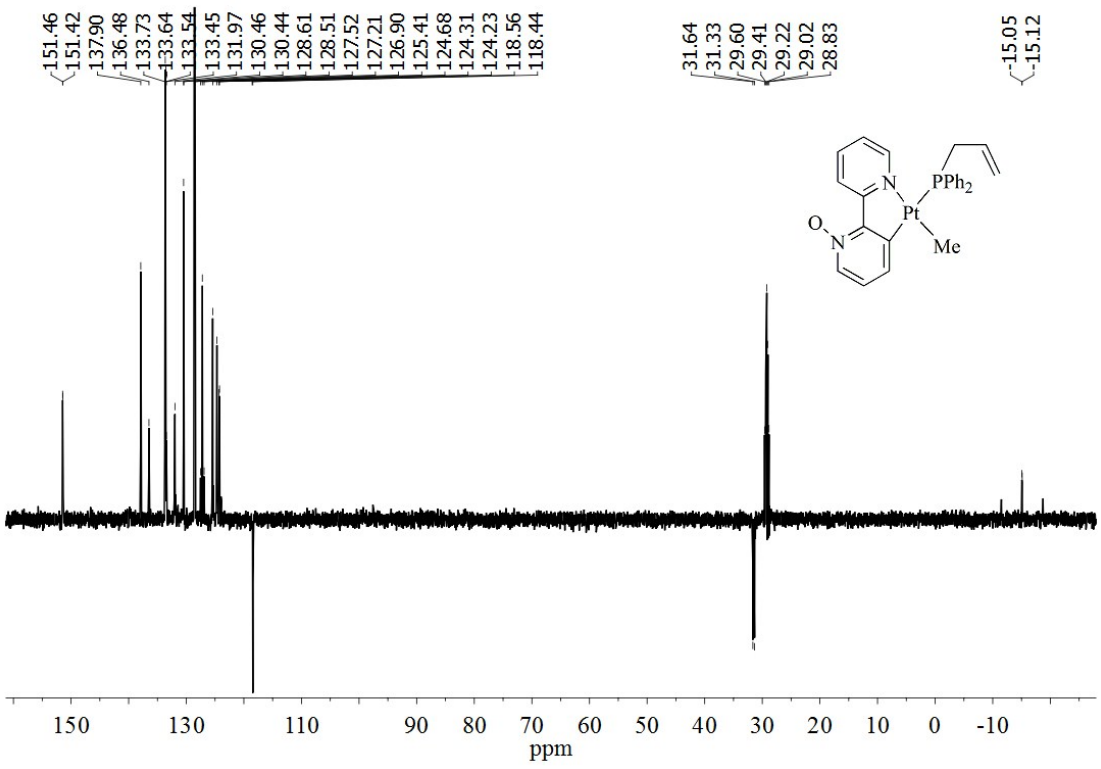


Figure S19. DEPT 135° spectrum of [Pt(O-bpy)(Me)(PPh$_2$allyl)], **3**, in acetone-d_6.

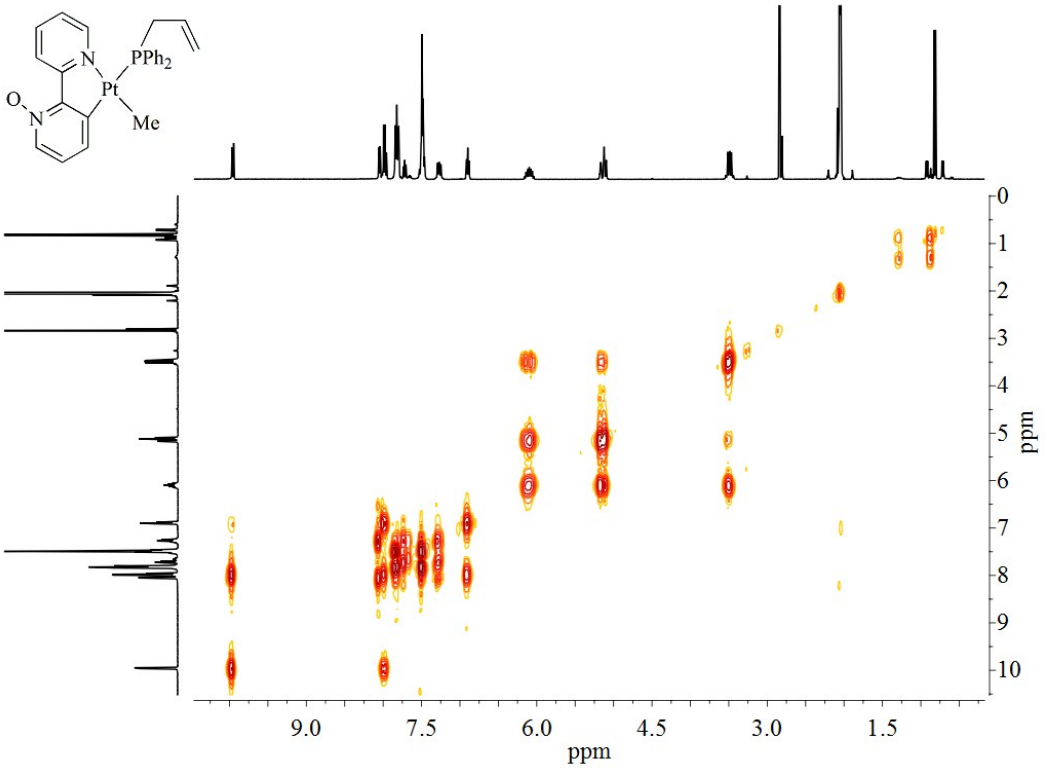


Figure S20. HHCOSY spectrum of [Pt(O-bpy)(Me)(PPh$_2$allyl)], **3**, in acetone-d_6.

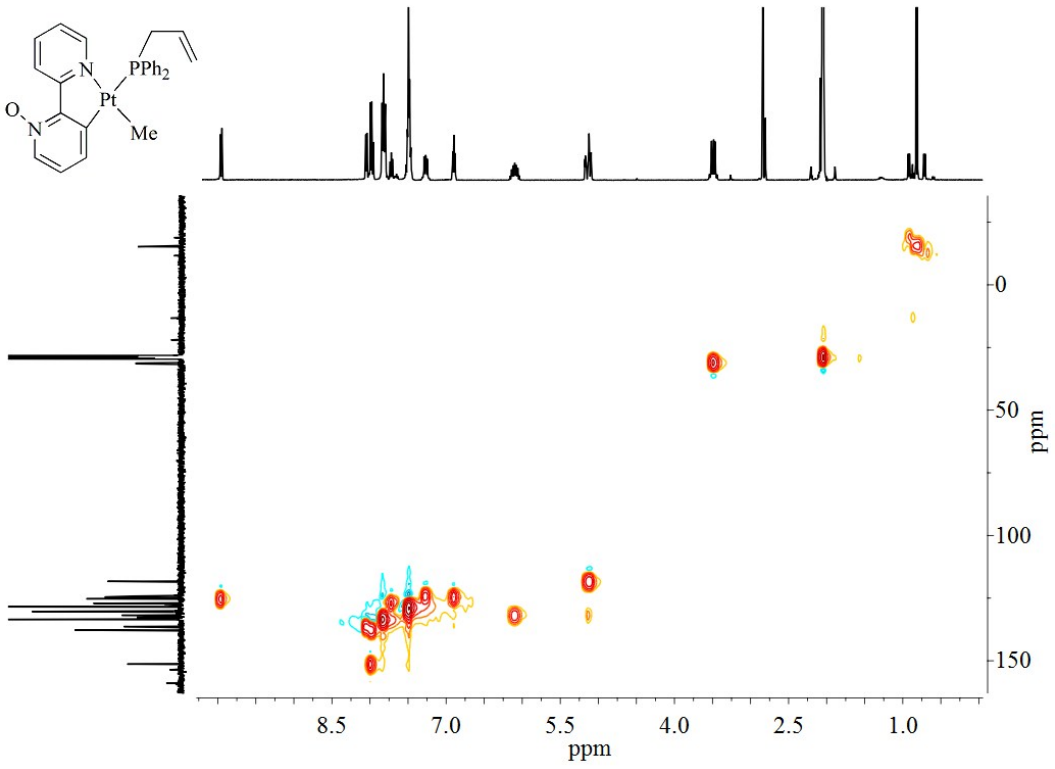


Figure S21. HSQC spectrum of [Pt(O-bpy)(Me)(PPh_2allyl)], **3**,in acetone-d_6.

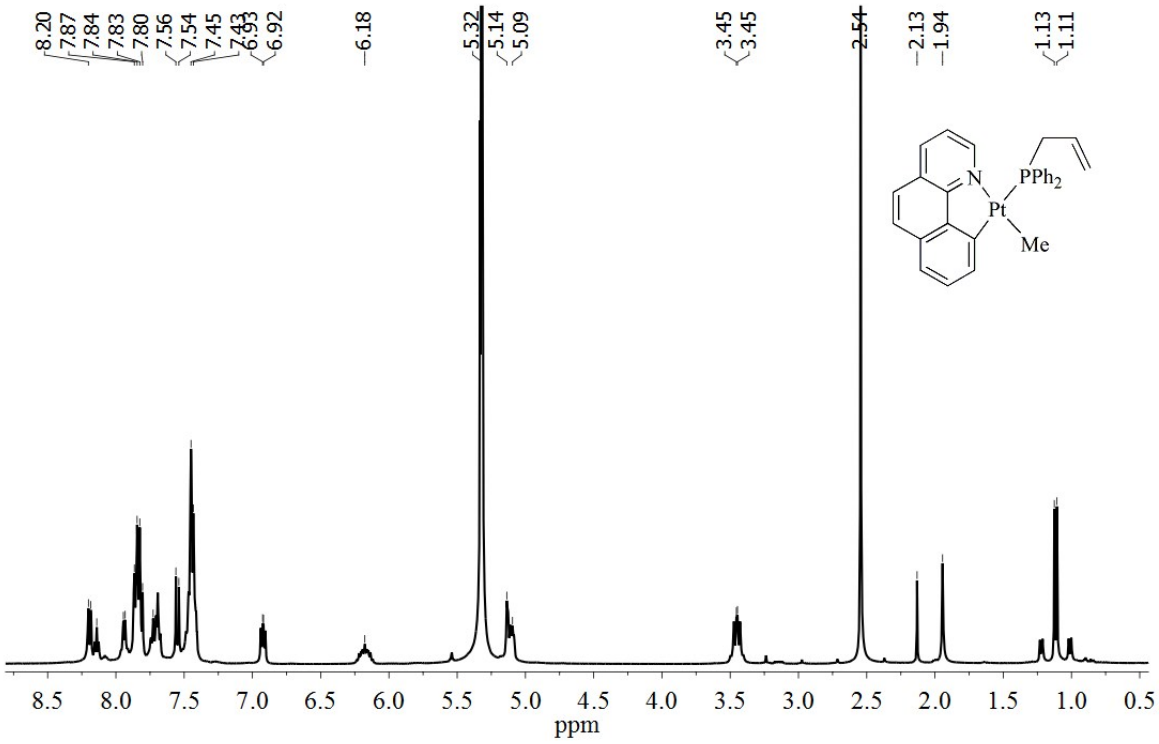


Figure S22. [1]HNMR spectrum of [Pt(bzq)(Me)(PPh_2allyl)], **4**, in CD_2Cl_2.

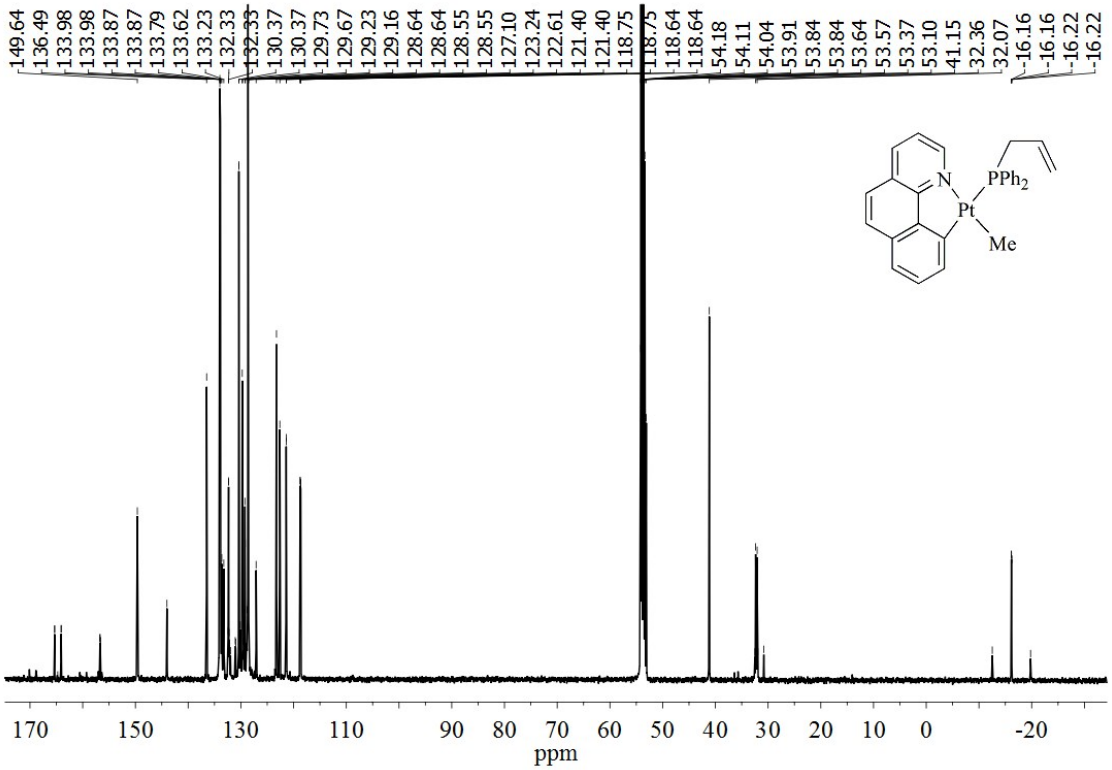


Figure S23. ^{13}CNMR spectrum of [Pt(bzq)(Me)(PPh$_2$allyl)], **4**, in CD_2Cl_2.

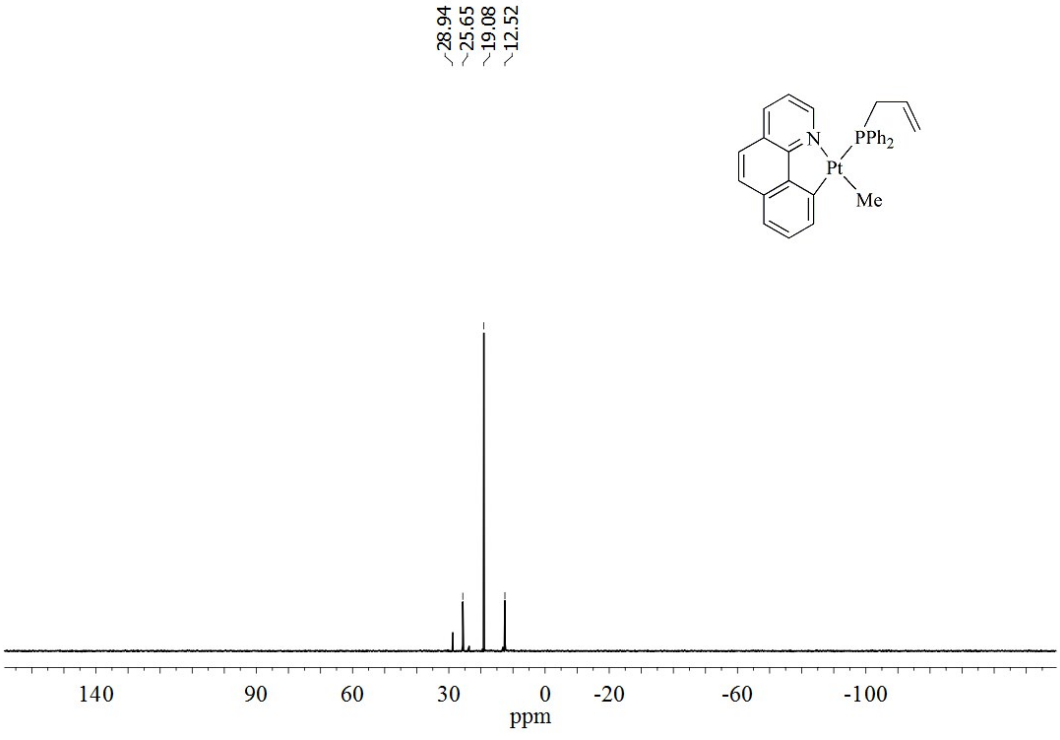


Figure S24. ^{31}PNMR spectrum of [Pt(bzq)(Me)(PPh$_2$allyl)], **4**, in CD_2Cl_2.

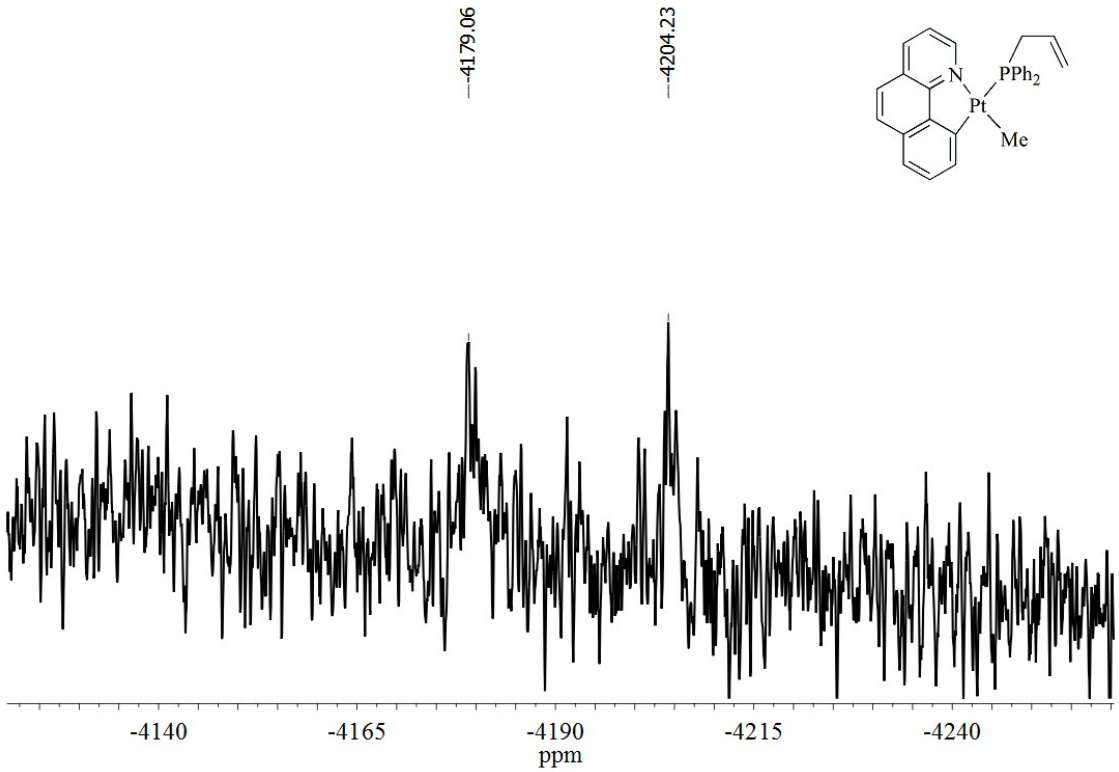


Figure S25. ^{195}PtNMR spectrum of [Pt(bzq)(Me)(PPh$_2$allyl)], **4**, in CD_2Cl_2.

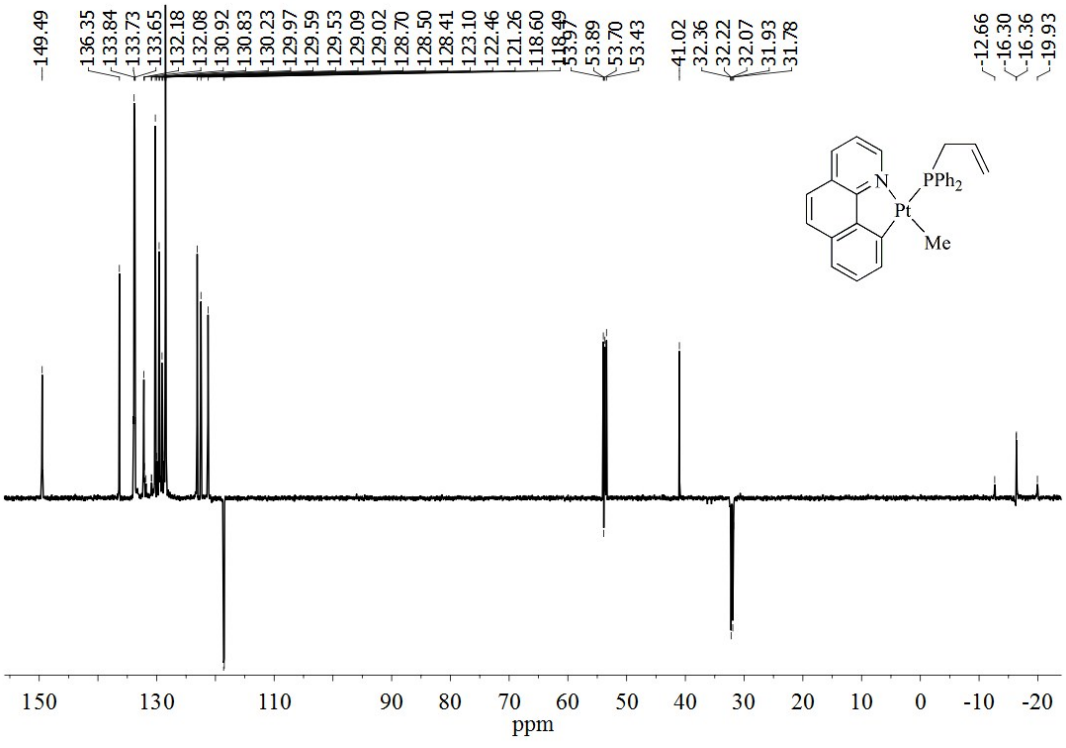


Figure S26. DEPT 135° spectrum of [Pt(bzq)(Me)(PPh$_2$allyl)], **4**, in CD_2Cl_2.

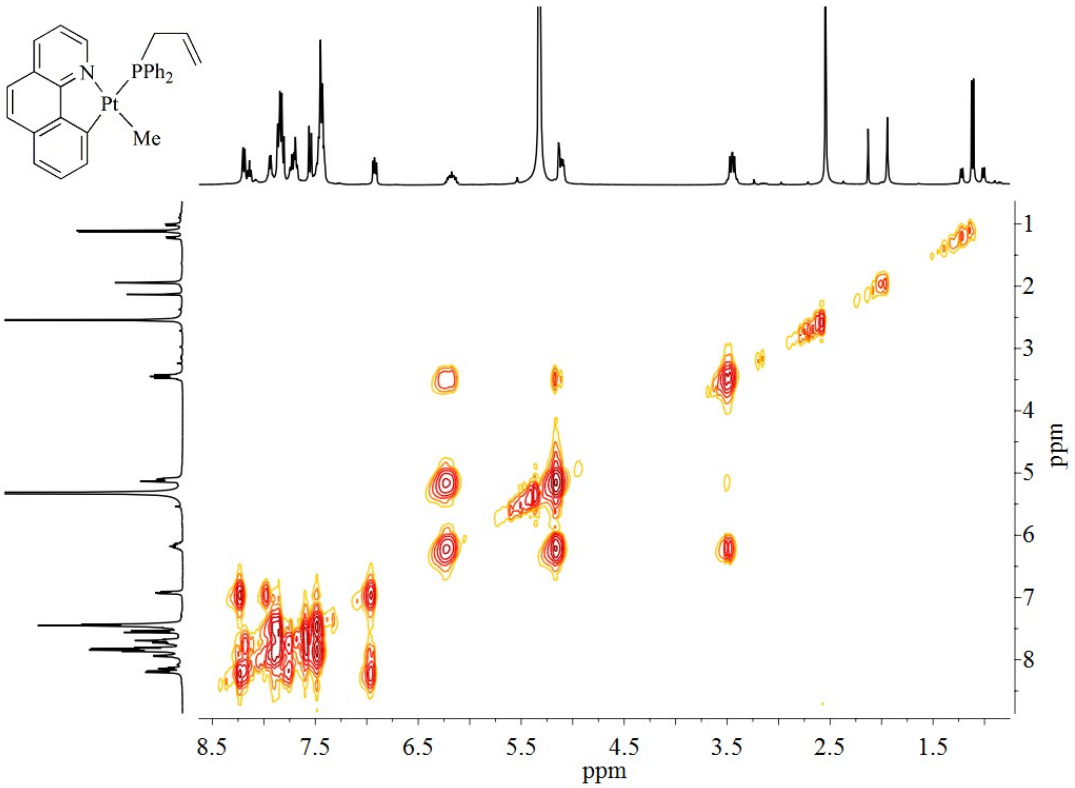


Figure S27. HHCOSY spectrum of [Pt(bzq)(Me)(PPh_2allyl)], **4**, in CD_2Cl_2.

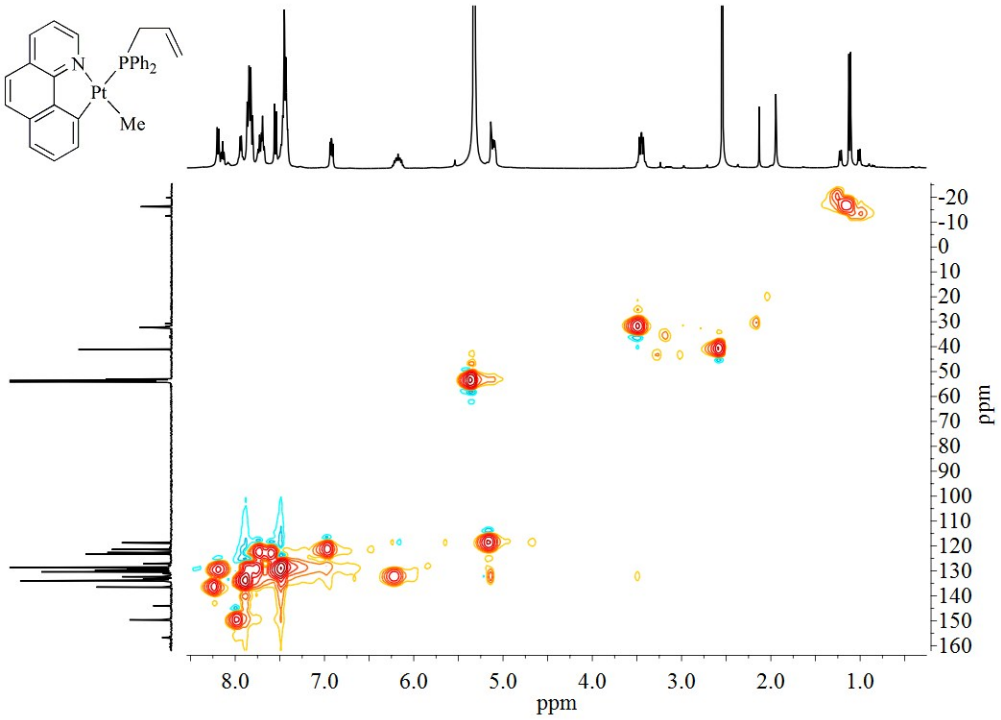


Figure S28. HSQC spectrum of [Pt(bzq)(Me)(PPh_2allyl)],**4** , in CD_2Cl_2.

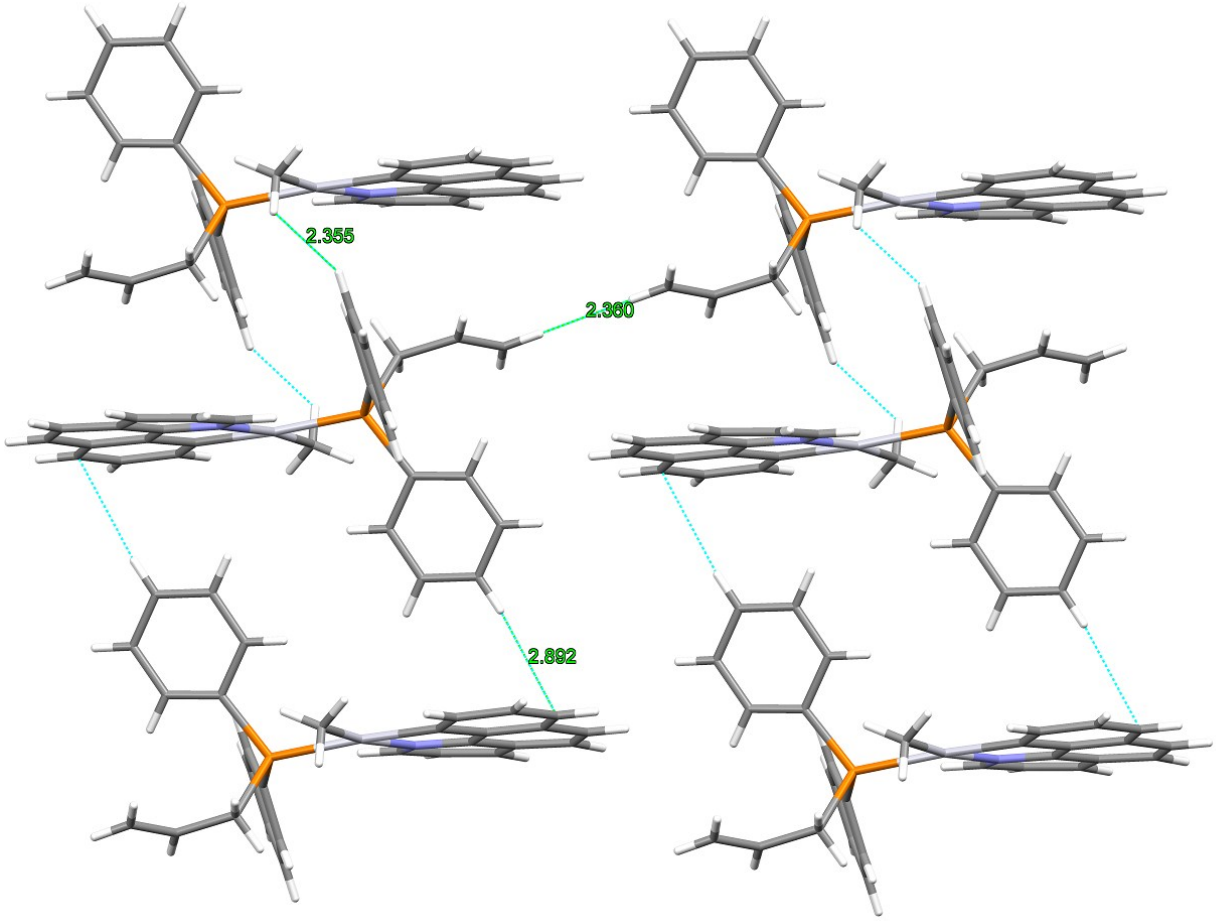


Figure S29. Crystal packing of the complex [Pt(bzq)(Me)(PPh_2allyl)], **4**, displaying the various intermolecular short contacts.

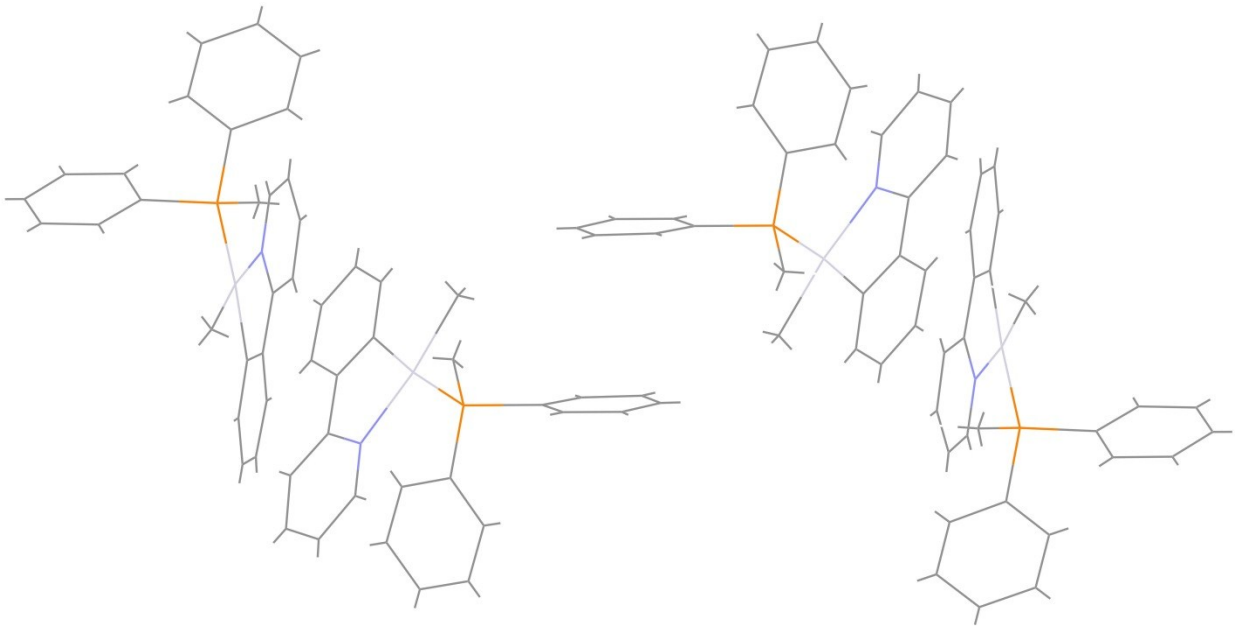


Figure S30. Crystal packing of the complex [Pt(ppy)(Me)(PPh_2Me)], **A** (obtained from the reference No. 47)

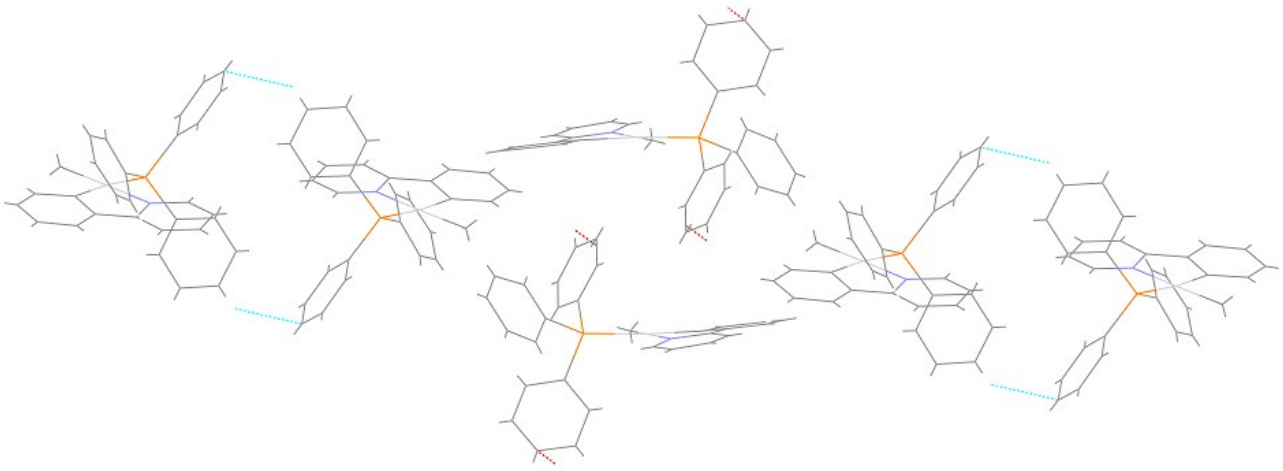


Figure S31. Crystal packing of the complex [Pt(ppy)(Me)(PPh_3)] B.

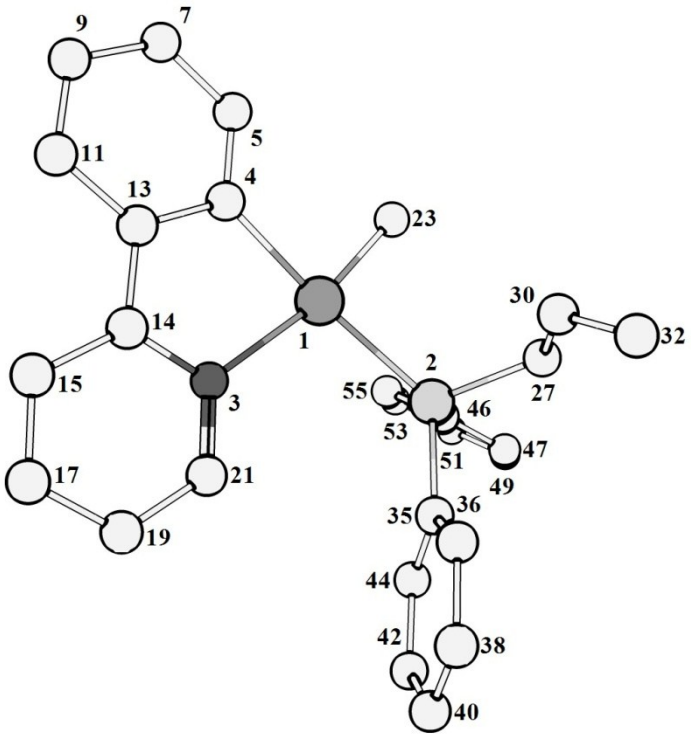


Figure S32. View of the DFT optimized structure of complex **1** with the atom numbering.

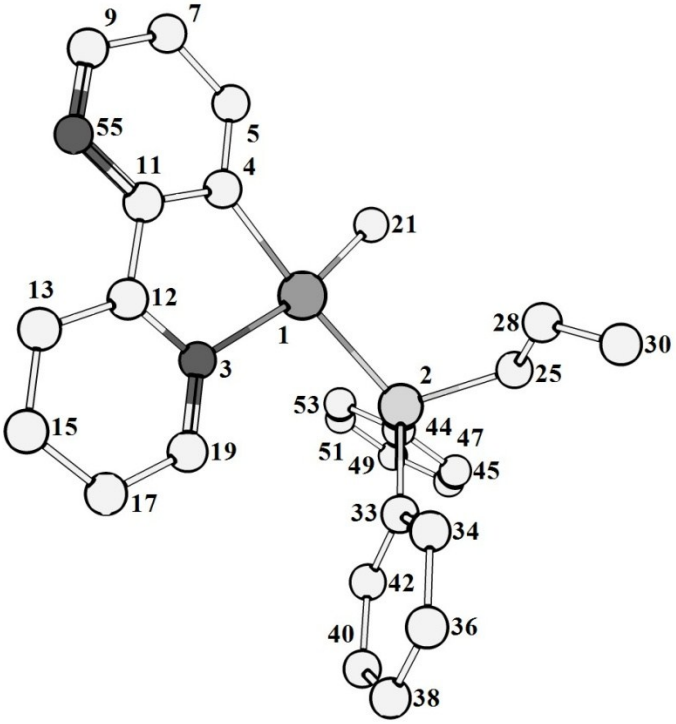


Figure S33. View of the DFT optimized structure of complex **2** with the atom numbering.

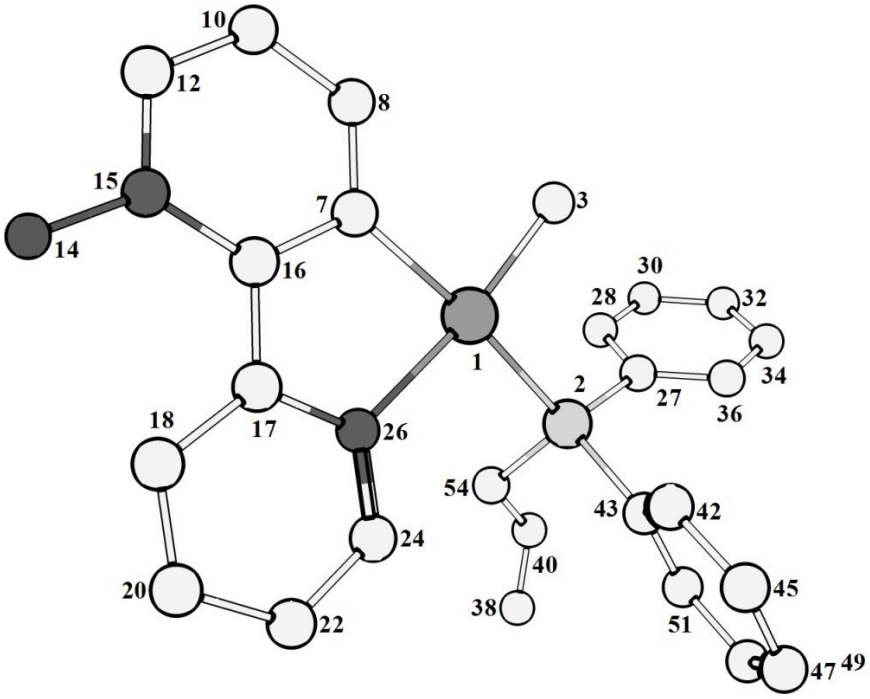


Figure S34. View of the DFT optimized structure of complex **3** with the atom numbering.

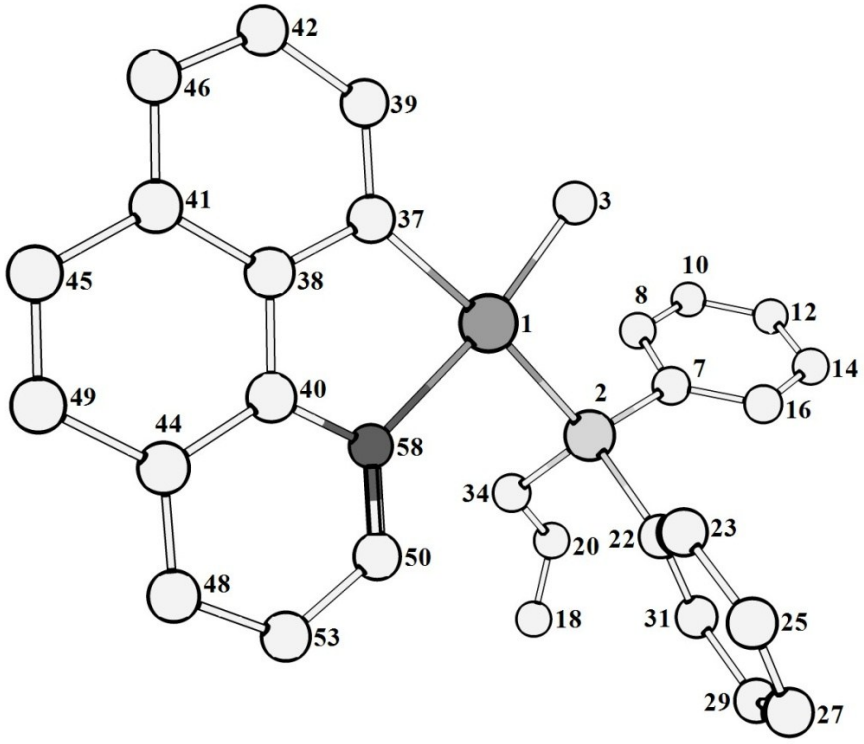


Figure S35. View of the DFT optimized structure of complex **4** with the atom numbering.

Table S1. Selected calculated bond distances (A°) and angles (deg) for the complex **1** (S_0 and T_1 states) compared with the corresponding experimental values.

Bond distance or angle	S_0	Crystal Stucture	T_1
Pt1-N3	2.20280	2.13619	2.15585
Pt1-C4	2.04720	2.03716	2.00717
Pt1-C23	2.08084	2.04017	2.09201
Pt1-P2	2.39643	2.30069	2.42017
P2-C27	1.88418	1.84875	1.88318
C27-C30	1.50243	1.46810	1.50078
C30-C32	1.33563	1.31069	1.33515
P2-C35	1.85129	1.81369	1.84790
P2-C46	1.84538	1.83152	1.84332
N3-C14	1.36332	1.35638	1.42302
C13-C14	1.46919	1.47044	1.39783
C13-C4	1.42157	1.36131	1.49127
N3-Pt1-P2	103.62776	105.18327	102.01457
P2-Pt1-C23	86.86748	83.89673	86.62891
C23-Pt1-C4	90.94158	92.22254	91.54861
C4-Pt1-N3	78.90334	78.72584	80.63349
N3-Pt1-C23	169.07009	170.91033	170.01240
P2-Pt1-C4	174.06889	175.33491	171.34891
Pt1-P2-C27	110.48767	114.26042	111.48789
P2-C27-C30	114.24361	114.58290	113.50718
C27-C30-C32	124.63049	124.28503	124.47559
Pt1-N3-C14	113.20335	113.10606	112.62759
N3-C14-C13	115.54026	116.05940	115.46760
C14-C13-C4	116.98537	115.22925	117.38267
C13-C4-Pt1	115.28408	116.56872	113.85168

Table S2. Selected calculated bond distances (A°) and angles (deg) for the complex **2** (S_0 and T_1 states).

Bond distance or angle	S_0	T_1
Pt1-N3	2.21979	2.17540
Pt1-C4	2.04511	2.00246
Pt1-C21	2.07859	2.08885
Pt1-P2	2.39151	2.42145
P2-C25	1.88361	1.88252
C25-C28	1.50244	1.50079
C28-C30	1.33555	1.33508
P2-C33	1.85024	1.84677
P2-C44	1.84466	1.84245
N3-C12	1.35752	1.41348
C12-C11	1.47313	1.39317
C11-C4	1.41515	1.48944
N3-Pt1-P2	103.31218	101.62212
P2-Pt1-C21	87.58083	87.21864
C21-Pt1-C4	90.33125	91.23217
C4-Pt1-N3	79.04489	80.66336
N3-Pt1-C21	168.80626	169.97716
P2-Pt1-C4	174.52096	171.88921
Pt1-P2-C25	110.63624	111.73587
P2-C25-C28	114.32777	113.46308
C25-C28-C30	124.61069	124.45793
Pt1-N3-C12	112.53960	111.91147
N3-C12-C11	115.77164	115.92532
C12-C11-C4	117.50517	117.84162
C11-C4-Pt1	115.09664	113.63369

Table S3. Selected calculated bond distances (A°) and angles (deg) for the complex **3** (S_0 state).

Bond distance or angle	S_0
Pt1-N26	2.20398
Pt1-C7	2.04598
Pt1-C3	2.07293
Pt1-P2	2.40909
P2-C54	1.88468
C54-C40	1.50156
C40-C38	1.33594
P2-C27	1.84472
P2-C42	1.84183
N26-C17	1.36752
C17-C16	1.47357
C16-C7	1.41985
N15-O14	1.29394
N26-Pt1-P2	98.92676
P2-Pt1-C3	91.02541
C3-Pt1-C7	92.08051
C7-Pt1-N26	78.60303
N26-Pt1-C3	169.36768
P2-Pt1-C7	171.37730
Pt1-P2-C54	107.80931
P2-C54-C40	118.80215
C54-C40-C38	124.43986
Pt1-N26-C17	114.42423
N26-C17-C16	113.52554
C17-C16-C7	118.34038
C16-C7-Pt1	114.92159
C16-N15-O14	123.37375
C12-N15-O14	117.20437

Table S4. Selected calculated bond distances (A°) and angles (deg) for the complex **4** (S_0 and T_1 states) compared with the corresponding experimental values.

Bond distance or angle	S_0	Crystal Structure	T_1
Pt1-N58	2.23854	2.15287	2.22469
Pt1-C37	2.04778	2.05678	2.02983
Pt1-C3	2.06576	2.03856	2.07046
Pt1-P2	2.39228	2.30181	2.40402
P2-C34	1.88765	1.84585	1.88499
C34-C20	1.50045	1.48303	1.50029
C20-C18	1.33578	1.30269	1.33569
P2-C22	1.84526	1.82021	1.84215
P2-C7	1.84675	1.83668	1.84541
N58-C40	1.36688	1.37484	1.34017
C40-C38	1.43451	1.41355	1.44659
C38-C37	1.42621	1.48714	1.40596
N58-Pt1-P2	97.14493	102.38729	96.90430
P2-Pt1-C3	92.94318	87.02961	92.72555
C3-Pt1-C37	90.92099	88.87436	91.76678
C37-Pt1-N58	79.38431	81.90531	79.09423
N58-Pt1-C3	169.56150	170.29587	170.04911
P2-Pt1-C37	172.23167	174.08600	170.33831
Pt1-P2-C34	107.68936	109.31459	107.34535
P2-C34-C20	119.24295	118.48960	118.78177
C34-C20-C18	124.70540	125.28530	124.60875
Pt1-N58-C40	110.86946	112.14388	111.18131
N58-C40-C38	117.04519	116.87756	117.15457
C40-C38-C37	118.71200	119.12987	117.73216
C38-C37-Pt1	113.92940	109.89896	114.73180

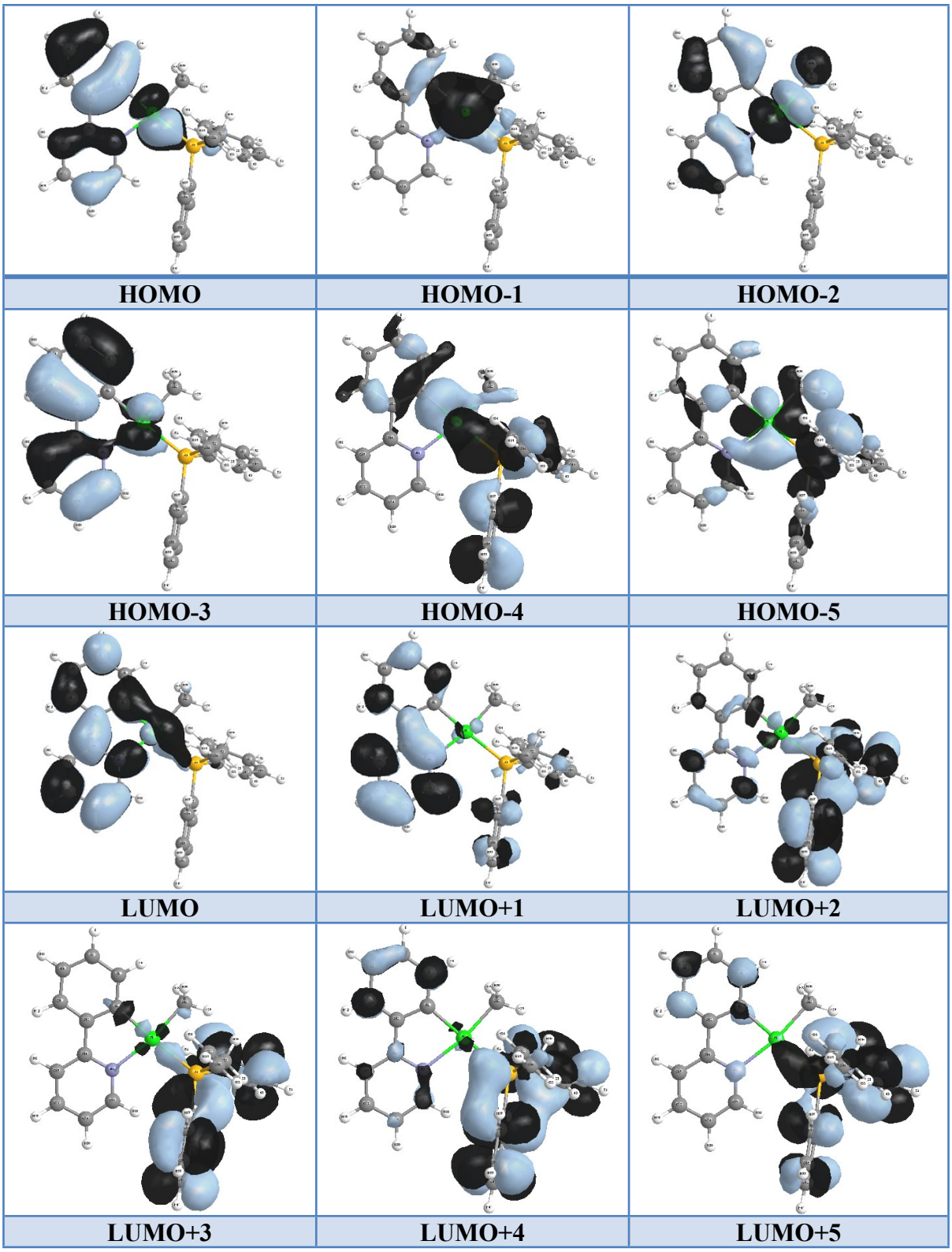


Figure S36. MO plots of the complex **1**.

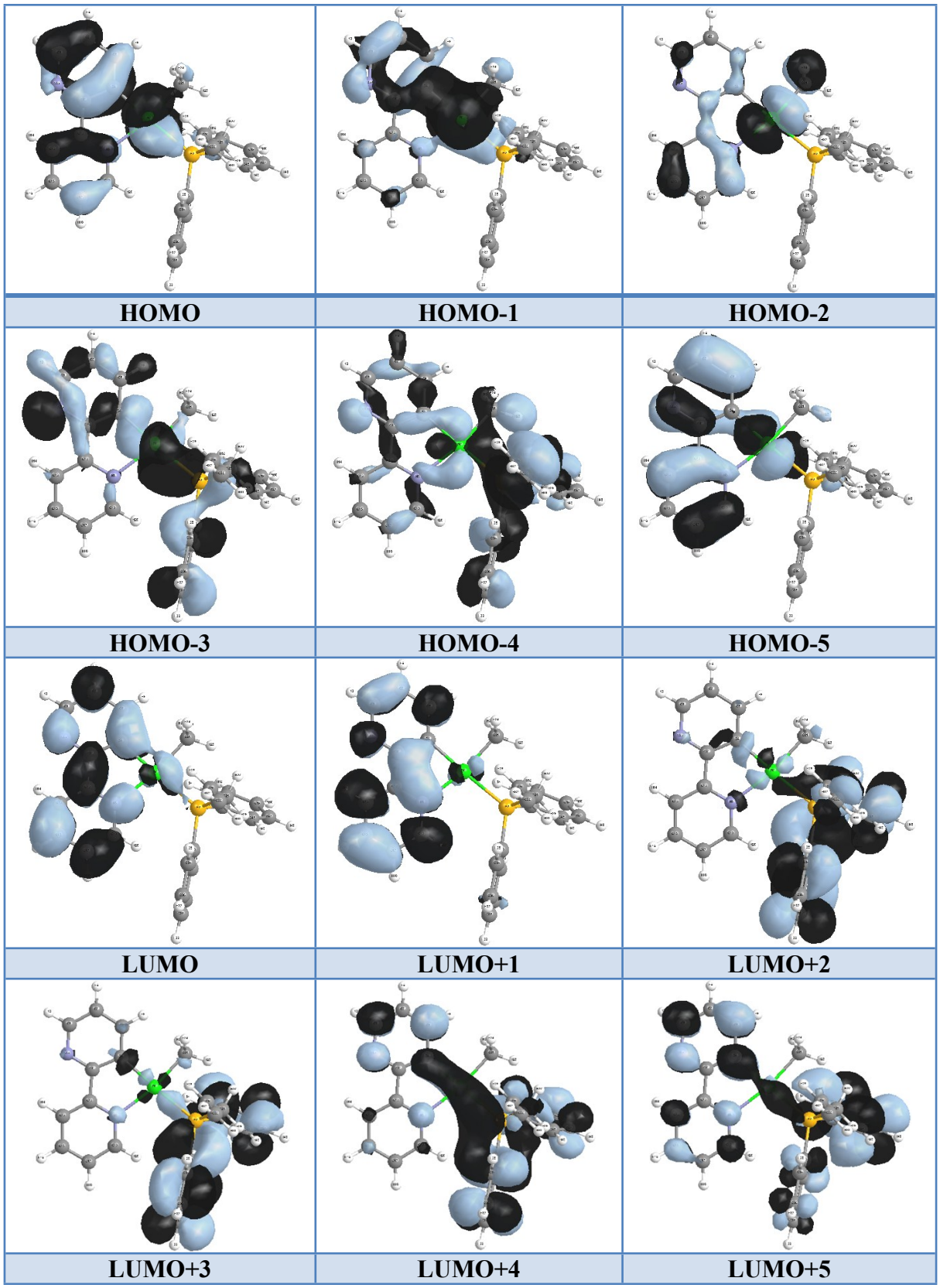
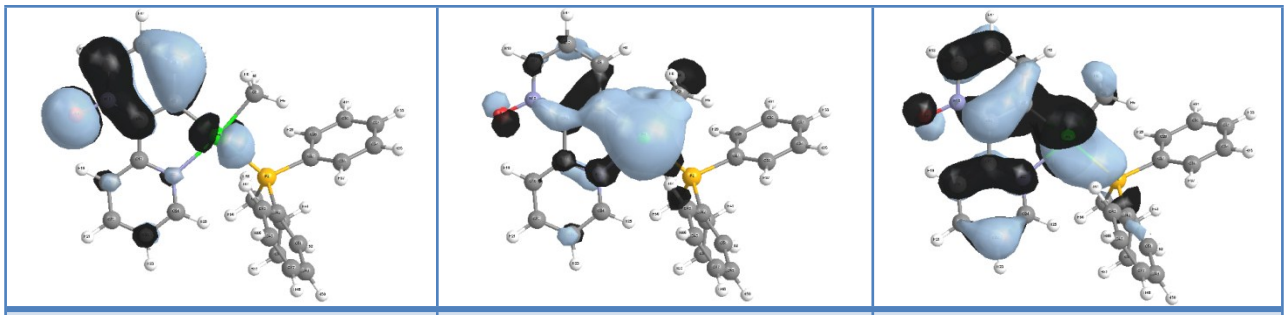
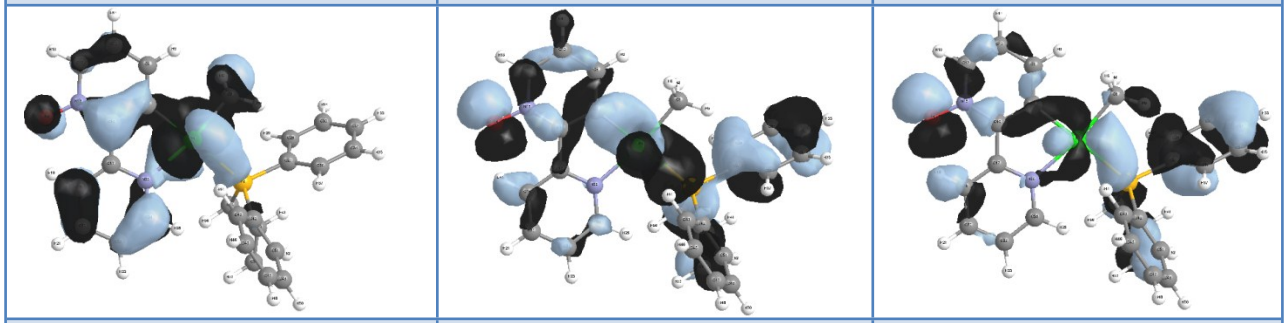


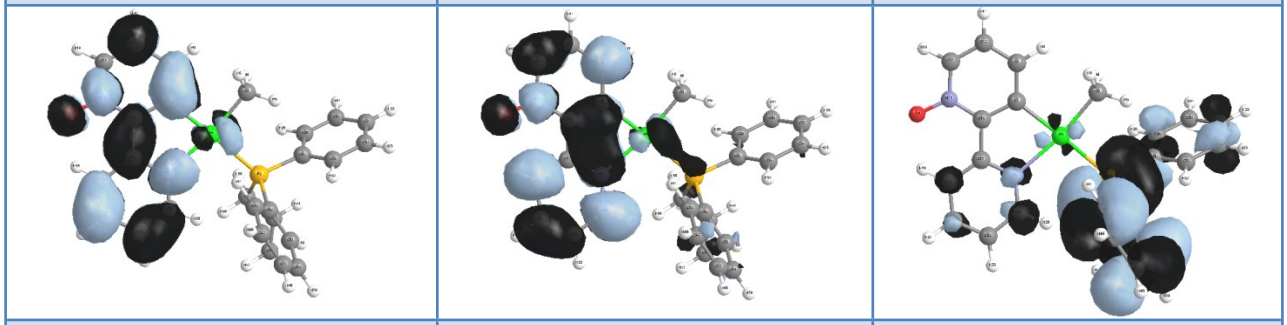
Figure S37. MO plots of the complex **2**.



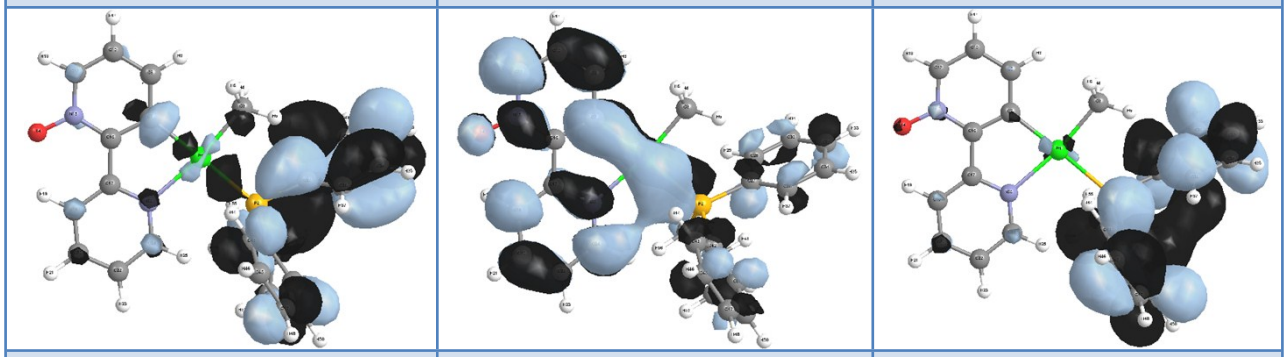
HOMO	HOMO-1	HOMO-2



HOMO-3	HOMO-4	HOMO-5



LUMO	LUMO+1	LUMO+2



LUMO+3	LUMO+4	LUMO+5

Figure S38. MO plots of the complex **3**.

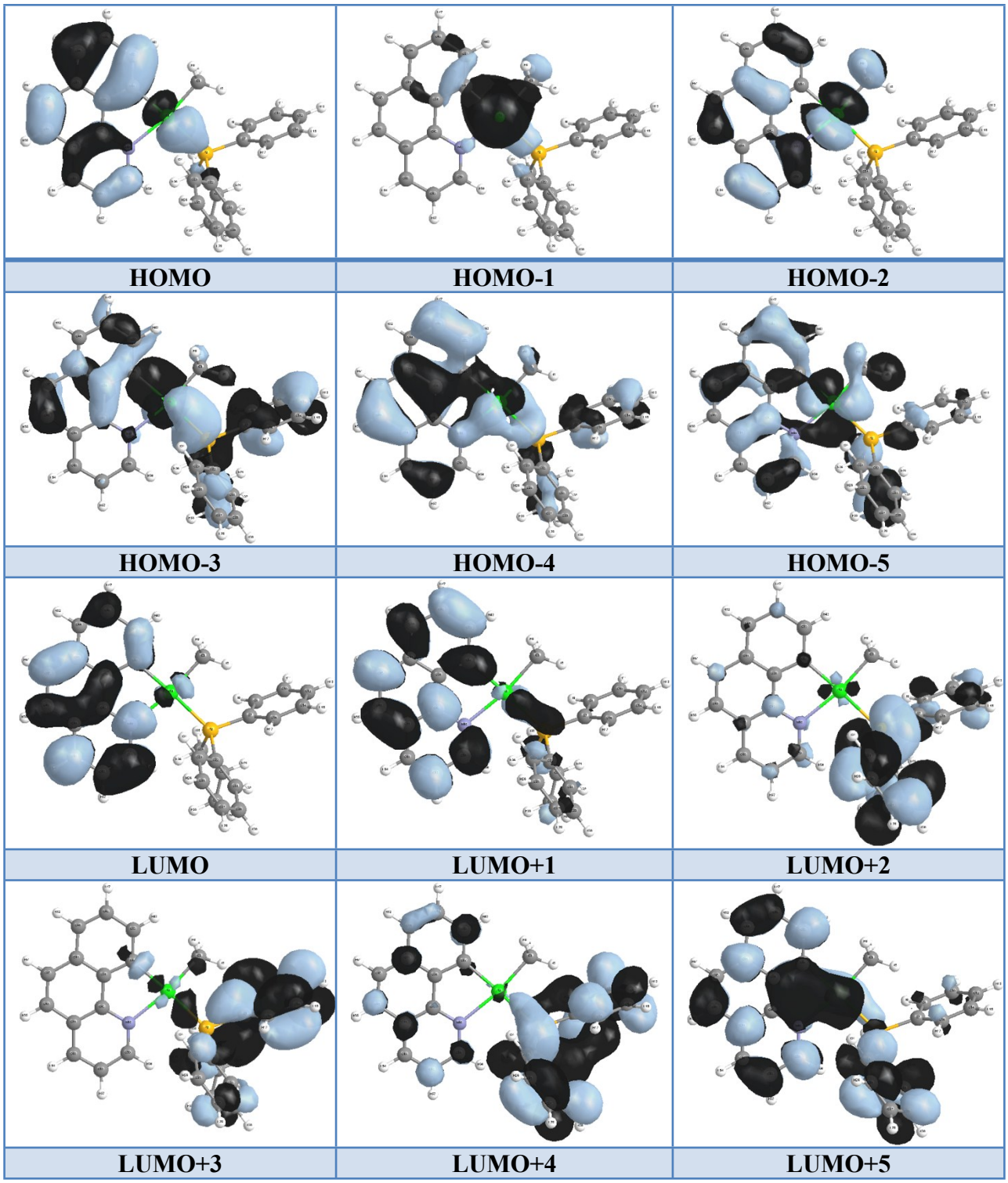


Figure S39. MO plots of the complex **4**.

Table S5. The energies of the selected molecular orbitals of complexes **1-4** and their compositions in singlet and triplet state (L´= allyldiphenylphosphane ligand).

		Complex 1					**Complex 2**				
		Energy	Components(%)				Energy	Components(%)			
State	MO	(eV)	Pt	L´	ppy	Me	(eV)	Pt	L´	bpy	Me
Singlet	LUMO+5	-0.192	4	87	8	1	-0.277	5	67	28	1
	LUMO+4	-0.475	5	86	10	0	-0.566	6	75	19	0
	LUMO+3	-0.684	9	85	5	1	-0.711	10	84	5	1
	LUMO+2	-0.781	8	83	9	0	-0.807	8	87	5	0
	LUMO+1	-0.856	2	14	83	0	-0.936	3	4	93	0
	LUMO	-1.489	6	5	89	0	-1.605	5	4	91	0
	HOMO	-5.701	46	4	50	0	-5.855	57	4	38	1
	HOMO-1	-5.820	83	5	9	3	-5.876	73	6	19	2
	HOMO-2	-6.067	80	5	14	1	-6.171	85	5	9	1
	HOMO-3	-6.311	21	2	77	0	-6.344	23	34	42	0
	HOMO-4	-6.440	15	56	29	0	-6.651	41	42	14	2
	HOMO-5	-6.657	65	23	9	3	-6.781	36	4	59	0
Triplet	HSOMO	-2.862	5	3	92	0	-3.032	5	2	93	0
	LSOMO	-5.685	44	3	52	1	-5.817	50	3	45	2
		Complex 3					**Complex 4**				
		Energy	Components(%)				Energy	Components(%)			
State	MO	(eV)	Pt	L´	O-bpy	Me	(eV)	Pt	L´	bzq	Me
Singlet	LUMO+5	-0.430	4	91	4	1	-0.180	6	33	61	0
	LUMO+4	-0.619	9	21	70	0	-0.475	6	80	14	0
	LUMO+3	-0.667	15	77	6	2	-0.613	15	79	5	1
	LUMO+2	-0.935	2	93	5	0	-0.859	1	93	6	0
	LUMO+1	-1.010	4	11	85	0	-1.157	3	14	82	0
	LUMO	-1.828	4	3	93	0	-1.674	3	3	94	0
	HOMO	-5.732	9	1	89	0	-5.575	33	4	63	0
	HOMO-1	-5.953	82	3	11	3	-5.837	85	4	8	3
	HOMO-2	-6.076	61	7	32	0	-6.007	75	4	20	1
	HOMO-3	-6.252	72	6	21	1	-6.367	22	41	36	1
	HOMO-4	-6.458	14	35	51	0	-6.431	23	18	59	0
	HOMO-5	-6.766	15	22	61	1	-6.679	59	19	20	2
Triplet	HSOMO	-	-	-	-	-	-2.928	1	2	97	0
	LSOMO	-	-	-	-	-	-5.618	44	7	49	0

Table S6. Wavelengths and corresponding nature of transitions for the complexes **1-4** where L = cyclometal ligands (ppy, bpy, O-bpy and bzq for the complexes **1**, **2**, **3** and **4** respectively), L′ = allyldiphenylphosphane ligand and L″ = Me ligand.

Complex	Calculated λ (nm)(*f*)	Transitions(Contribution)	Assignment
1	362 (0.028)	HOMO→LUMO (0.66)	ILCT/MLCT
		HOMO-1→LUMO (0.20)	MLCT
	357 (0.017)	HOMO-1→LUMO (0.67)	MLCT
		HOMO→LUMO (0.19)	ILCT/MLCT
	324 (0.110)	HOMO-2→LUMO (0.67)	MLCT/ILCT
		HOMO→LUMO (0.12)	ILCT/MLCT
	302 (0.037)	HOMO→LUMO+1 (0.52)	ILCT/MLCT/ML′CT
		HOMO-3→LUMO (0.41)	ILCT/MLCT
		HOMO→LUMO+2 (0.10)	ML′CT/LL′CT
		HOMO-2→LUMO (0.10)	MLCT/ILCT
	287 (0.122)	HOMO-3→LUMO (0.40)	ILCT/MLCT
		HOMO→LUMO+1 (0.35)	ILCT/MLCT/ML′CT
		HOMO-5→LUMO (0.33)	L′LCT/MLCT
		HOMO-1→LUMO+2 (0.15)	ML′CT/LL′CT
		HOMO-2→LUMO+1 (0.14)	ILCT/MLCT/ML′CT
2	365 (0.008)	HOMO-1→LUMO (0.58)	MLCT/ILCT
		HOMO→LUMO (0.40)	ILCT/MLCT
	356 (0.031)	HOMO→LUMO (0.55)	ILCT/MLCT
		HOMO-1→LUMO (0.39)	MLCT/ILCT
		HOMO-2→LUMO (0.16)	MLCT/ILCT
	325 (0.107)	HOMO-2→LUMO (0.66)	MLCT/ILCT
		HOMO-3→LUMO (0.14)	MLCT/ILCT/L′LCT
		HOMO→LUMO (0.13)	ILCT/MLCT
	321 (0.014)	HOMO-3→LUMO (0.65)	MLCT/ILCT/L′LCT
		HOMO-4→LUMO (0.16)	MLCT/ILCT/L′LCT
		HOMO-2→LUMO (0.14)	MLCT/ILCT
		HOMO-1→LUMO+1 (0.11)	ILCT/MLCT
	293 (0.041)	HOMO→LUMO+1 (0.52)	ILCT/MLCT
		HOMO-1→LUMO+1 (0.38)	ILCT/MLCT
		HOMO-5→LUMO (0.20)	ILCT/MLCT
3	379 (0.013)	HOMO-1→LUMO (0.64)	MLCT/ILCT
		HOMO→LUMO (0.27)	ILCT/MLCT
	373 (0.069)	HOMO→LUMO (0.55)	ILCT/MLCT
		HOMO-2→LUMO (0.33)	ILCT/MLCT/L′LCT
		HOMO-1→LUMO(0.25)	MLCT/ILCT
	359 (0.046)	HOMO-2→LUMO (0.58)	ILCT/MLCT/L′LCT
		HOMO→LUMO (0.29)	ILCT/MLCT
		HOMO-3→LUMO (0.20)	ILCT/MLCT
		HOMO-1→LUMO (0.11)	MLCT/ILCT
	330 (0.098)	HOMO-3→LUMO (0.56)	ILCT/MLCT
		HOMO-4→LUMO (0.29)	ILCT/MLCT/L′LCT
		HOMO-5→LUMO (0.18)	ILCT/MLCT/L′LCT
		HOMO-2→LUMO (0.15)	ILCT/MLCT/L′LCT
		HOMO-2→LUMO+1 (0.12)	ILCT/MLCT
	284 (0.096)	HOMO-2→LUMO+1 (0.56)	ILCT/MLCT
		HOMO-3→LUMO+1 (0.24)	ILCT/MLCT
		HOMO→LUMO+1 (0.22)	ILCT/MLCT/L′LCT
		HOMO-1→LUMO+1 (0.11)	MLCT/ILCT

4	385 (0.040)	HOMO→LUMO (0.67)	ILCT/MLCT
		HOMO-2→LUMO (0.14)	ILCT/MLCT
		HOMO-1→LUMO (0.10)	MLCT
	368 (0.009)	HOMO-1→LUMO (0.69)	MLCT
	342 (0.060)	HOMO-2→LUMO (0.62)	ILCT/MLCT
		HOMO→LUMO+1 (0.23)	ILCT/MLCT/ML′CT
		HOMO-2→LUMO+1 (0.16)	ILCT/MLCT/ML′CT
		HOMO→LUMO (0.15)	ILCT/MLCT
	324 (0.188)	HOMO→LUMO+1 (0.61)	ILCT/MLCT/ML′CT
		HOMO-4→LUMO (0.22)	ILCT/MLCT/L′LCT
		HOMO-2→LUMO (0.20)	ILCT/MLCT
		HOMO-3→LUMO (0.15)	ILCT/MLCT/L′LCT
	306 (0.053)	HOMO-2→LUMO+1 (0.52)	ILCT/MLCT/ML′CT
		HOMO-3→LUMO (0.30)	ILCT/MLCT/L′LCT
		HOMO-4→LUMO (0.23)	ILCT/MLCT/L′LCT
		HOMO-2→LUMO (0.19)	ILCT/MLCT
		HOMO→LUMO+1 (0.13)	ILCT/MLCT/ML′CT
	285 (0.081)	HOMO-6→LUMO (0.38)	ILCT/MLCT/L′LCT
		HOMO-4→LUMO+1 (0.34)	ILCT/MLCT/L′LCT
		HOMO-3→LUMO+1 (0.25)	ILCT/MLCT/L′LCT

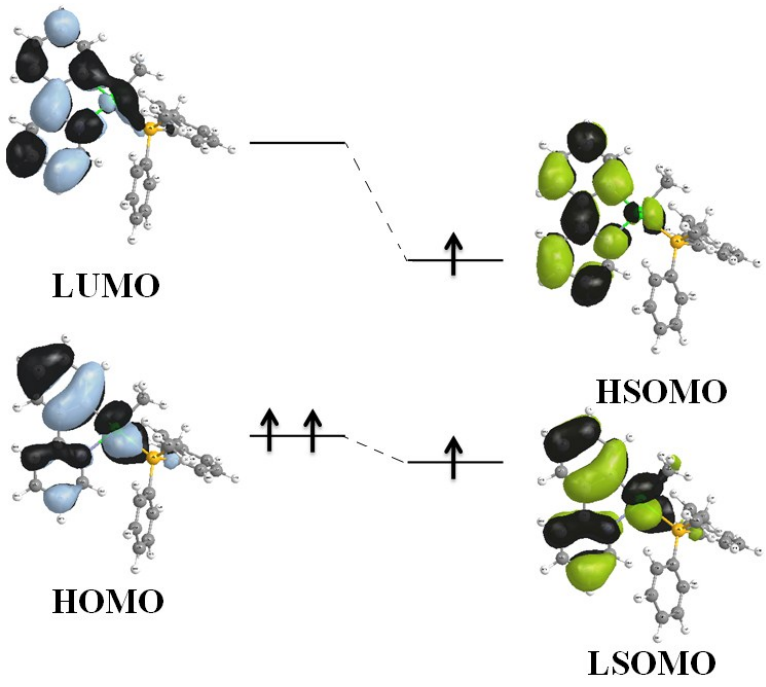


Figure S40. Comparitive MO diagram for computed S_0 (left) and T_1 (right) states of the complex **1**.

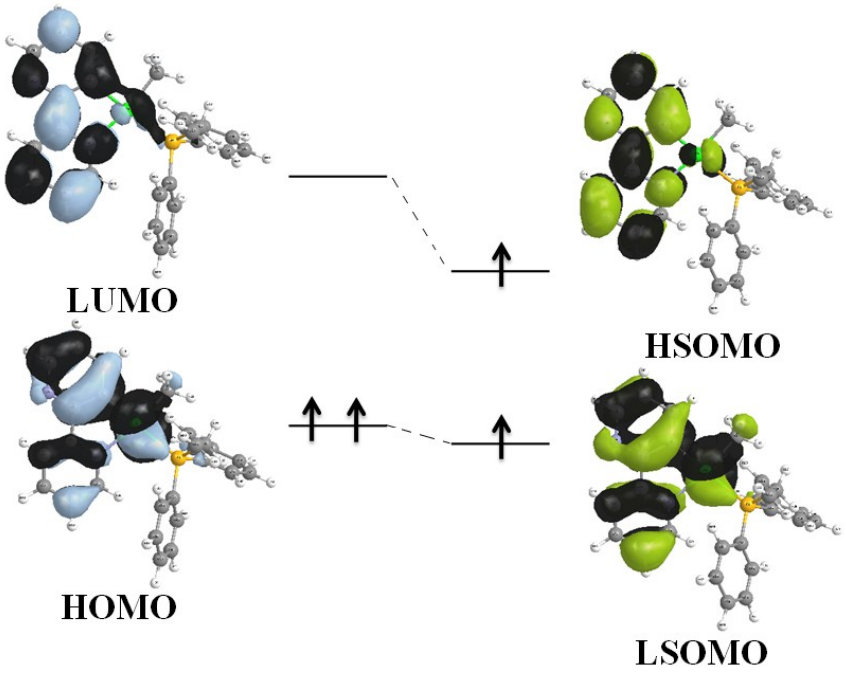


Figure S41. Comparitive MO diagram for computed S_0 (left) and T_1 (right) states of the complex **2**.

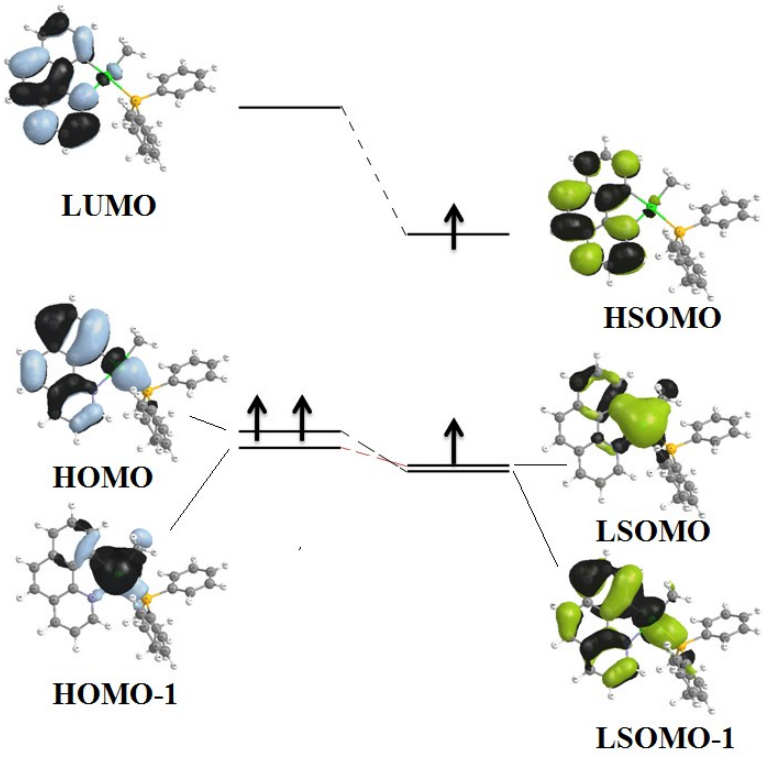


Figure S42. Comparitive MO diagram for computed S_0 (left) and T_1 (right) states of the complex **4**.

Table S7. Crystallographic and structure refinement data for the complexes **1**, **4** and **B**.

	Complex 1	**Complex 4**	**Complex B**
Empirical formula	$C_{27}H_{26}NPPt$	$C_{29}H_{26}NPPt$	$C_{30}H_{26}NPPt$
Formula weight	590.54	614.56	626.57
Temperature	298(2) K	298(2) K	298(2) K
Wavelength	0.71073 A	0.71073 A	0.71073 A
Crystal system, space group	Monoclinic, *P21/n*	Triclinic, $P\bar{1}$	Monoclinic, $P2_1/c$
Unit cell dimensions	a = 9.759(2) A alpha = 90 deg. b = 10.351(2) A beta = 100.86(3)deg. c = 23.222(5) A gamma = 90 deg.	a = 9.1117(18) A alpha = 95.86(3) deg. b = 11.229(2) A beta = 103.50(3) deg. c = 12.539(3) A gamma =102.41(3) deg.	a = 9.6029(19) A alpha = 90 deg. b = 13.097(3) A beta = 100.17(3)deg. c = 19.630(4) A gamma = 90 deg.
Volume	2303.8(8) A^3	1202.6(4) A^3	2430.1(9) A^3
Z, Calculated density	4, 1.703 Mg/m^3	2, 1.697 Mg/m^3	4, 1.713 Mg/m^3
Absorption coefficient	6.174 mm^-1	5.917 mm^-1	5.859 mm^-1
F(000)	1152	600	1224
Crystal size	0.45 x 0.20 x 0.15 mm	0.45 x 0.40 x 0.30 mm	0.25 x 0.30 x 0.50 mm
Theta range for data collection	2.14 to 25.00 deg.	2.32 to 25.00 deg.	2.10 to 25.00 deg.
Limiting indices	-11<=h<=11, -11<=k<=12, -27<=l<=27	-10<=h<=10, -13<=k<=12, -14<=l<=14	-11<=h<=8, -15<=k<=14, -23<=l<=23
Reflections collected / unique	10787 / 4041 [R(int) = 0.0677]	8788 / 4210 [R(int) = 0.0944]	11136 / 4265 [R(int) = 0.089]
Absorption correction	Numerical	Numerical	Numerical
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	4041 / 0 / 230	4210 / 0 / 290	4265 / 0 / 299
Goodness-of-fit on F^2	0.926	0.952	0.869
Final R indices [I>2sigma(I)]	R1 = 0.0458, wR2 = 0.0987	R1 = 0.0424, wR2 = 0.0952	R1 = 0.0397, wR2 = 0.0828
R indices (all data)	R1 = 0.0777, wR2 = 0.1159	R1 = 0.0546, wR2 = 0.0982	R1 = 0.0730, wR2 = 0.0952
CCDC No.	1509609	1509608	1538745