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Electronic Supplementary Information

Coligand driven diverse organometallation in hydrazone-derivatized pyrene: ortho vs peri C–H activation

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Table S1 Crystallographic details of **2a**, **3a** and **3b**

	2a.CH_2Cl_2	**3a.1.5CH_2Cl_2**	**3b. CH_2Cl_2**
Empirical formula	$C_{62}H_{46}Cl_3N_3OP_2Ru$ S	$C_{62.50}H_{46}Cl_3N_3OP_2RuS$	$C_{60}H_{45}Cl_2N_3OP_2RuS$
fw	1150.44	1156.44	1089.96
T /K	296(2)K	296(2)K	273(2)K
Crystal system	Triclinic	Triclinic	orthorhombic
Space group	$P\,\bar{1}$	$P\,\bar{1}$	*P b c a*
a / Å	12.4913(5)	9.8421(7)	11.2036(9)
b / Å	13.6943(5)	11.9671(8)	23.8440(19)
c / Å º	17.6253(7)	24.6276(18)	37.483(3)
α /deg	74.404(2)	77.378(3)	90
β / deg	83.684(2)	78.715(3)	90
γ / deg	67.309(2)	66.813(3)	90
V /Å^3	2679.13(19)	2582.4(3)	10013.2(14)
Z	2	2	8
D_c /Mgm^{-3}	1.426	1.487	1.446
μ /mm^{-1}	0.587	0.609	0.572
F(000)	1176	1182	4464
cryst size/mm^3	0.2×0.1×0.05	0.04×0.03×0.02	0.04×0.03×0.02
θ/deg	1.767–27.525	0.855–26.00	1.708-24.998
measured reflns	45515	31382	118913
unique reflns/R_{int}	12246/ 0.0366	9532/ 0.0619	8817/0.1219
[a]GOF on F^2	1.028	1.062	1.117
[b]R1, wR2[c] [$I > 2\sigma(I)$]	0.0398, 0.1012	0.0817, 0.1502	0.0447, 0.0978
R1, wR2	0.0531, 0.1098	0.1291, 0.1766	0.0938, 0.1318

[a]GOF = $\{\Sigma[w(F_o^2-F_c^2)^2]/(n-p)\}^{1/2}$. [b]R1 = $\Sigma||F_o|-|F_c||/\Sigma|F_o|$.

[c]wR2 = $[\Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]]^{1/2}$ where $w = 1/[\sigma^2(F_o^2)+(aP)^2+bP]$, $P = (F_o^2+2F_c^2)/3$.

Table S2 Crystallographic details of **4a** and **5a**

	4a	**5a**
Empirical formula	$C_{61}H_{45}N_3OP_2RuS$	$C_{61}H_{43}N_3OP_2RuS$
fw	1031.07	1029.05
T /K	151(2)K	273(2)K
Crystal system	Triclinic	Triclinic
Space group	$P\bar{1}$	$P\bar{1}$
a / Å	10.6241(5)	9.6836(12)
b / Å	13.8517(8)	12.2483(15)
c / Å º	17.2984(8)	21.905(3)
α /deg	96.521(4)	86.801(3)
β / deg	104.809(4)	86.645(3)
γ / deg	96.619(4)	67.402(3)
V /Å^3	2417.6(6)	2393.0(5)
Z	2	2
D_c /Mgm^{-3}	1.416	1.428
μ /mm^{-1}	0.481	0.486
F(000)	1060	1056
cryst size/mm^3	0.17×0.10×0.05	0.06×0.04×0.02
θ/deg	2.0340–29.0280	1.802–27.166
measured reflns	8463	72090
unique reflns/R_{int}	6491/ 0.0943	10573/ 0.1030
[a]GOF on F^2	1.021	1.131
[b]R1, wR2[c] [$I > 2\sigma(I)$]	0.0600, 0.1417	0.0958, 0.2130
R1, wR2	0.0794, 0.1555	0.1249, 0.2278

[a]GOF = $\{\Sigma[w(F_o^2-F_c^2)^2]/(n-p)\}^{1/2}$. [b]R1 = $\Sigma||F_o|-|F_c||/\Sigma|F_o|$.
[c]wR2 = $[\Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]]^{1/2}$ where $w = 1/[\sigma^2(F_o^2)+(aP)^2+bP]$, $P = (F_o^2+2F_c^2)/3$.

Table S3 Selected experimental and theoretical bond parameters of **2a, 3a** and **3b**

	2a			**3a**			**3b**	
	Expt.	**Theo.**		**Expt.**	**Theo.**		**Expt.**	**Theo.**
Ru1–N1	2.189(2)	2.33439	Ru1–N1	2.152(5)	2.232	Ru1–N1	2.161(4)	2.23286
Ru1–N2	2.129(19)	2.15020	Ru1–N3	2.072(4)	2.096	Ru1–N3	2.057(4)	2.09695
Ru1–C25	1.909(4)	1.83969	Ru1–C25	1.856(5)	1.876	Ru1–C23	1.822(5)	1.87637
Ru1–Cl1	2.3965(7)	2.48034	Ru1–C21	2.107(5)	2.117	Ru1–C18	2.105(4)	2.11722
Ru1–P1	2.3814 (6)	2.50014	Ru1–P1	2.418(14)	2.513	Ru1–P1	2.404(12)	2.51322
Ru1–P2	2.3952(11)	2.47595	Ru1–P2	2.410(14)	2.517	Ru1–P2	2.412(12)	2.51706
N1–C7	1.325(3)	1.33271	N1–C7	1.336(7)	1.345	N1–C7	1.327(6)	1.34538
N2–C7	1.331(3)	1.33419	N2–C7	1.312(7)	1.322	N2–C7	1.327(6)	1.32264
N2–N3	1.356(3)	1.34247	N2–N3	1.396(6)	1.381	N2–N3	1.403(5)	1.38120
N3–C8	1.281(3)	1.29546	N3– C8	1.300(7)	1.302	N3–C8	1.294(6)	1.30237
C8–C9	1.460(3)	1.45884	C8–C9	1.451(8)	1.442	C8–C9	1.445(6)	1.44297
C1–C6	1.397(4)	1.41970	C21–C22	1.466(7)	1.457	C18–C19	1.450(6)	1.45773
C25–O1	0.990(4)	1.16280	C25–O1	1.144(6)	1.166	C23–O1	1.176(6)	1.16623
N1–Ru1–N2	61.63(7)	60.02328	N1–Ru1–N3	75.65(17)	75.954	N1–Ru1–N3	76.78(15)	75.954
C25−Ru1−N2	101.57(10)	101.46520	N3–Ru1–C21	90.84(18)	89.350	N3–Ru1–C18	89.72(16)	89.350
C25−Ru1−Cl1	100.61(8)	90.81956	C21–Ru1–C25	94.80(2)	96.364	C18–Ru1–C23	96.44(18)	96.364
N1–Ru1–C25	163.16(9)	161.45183	N1–Ru1–C25	98.90(2)	98.545	N1–Ru1–C23	97.35(17)	98.545
P1–Ru1–P2	177.36(2)	177.21645	P1–Ru1–P2	176.87(5)	174.592	P1–Ru1–P2	174.49(5)	174.592

Table S4 Selected experimental and theoretical bond parameters of **4a** and **5a**

	4a			**5a**	
	Expt.	**Theo.**		**Expt.**	**Theo.**
Ru1–N1	2.116(3)	2.16335	Ru1–N1	2.168(7)	2.24758
Ru1–N3	2.182(4)	2.24888	Ru1–N3	2.051(5)	2.08929
Ru1–C25	1.823(5)	1.86179	Ru1–C25	1.858(7)	1.88713
Ru1–H1	1.67(4)	1.62077	Ru1–C10	2.100(8)	2.11734
Ru1–P1	2.3614(11)	2.44172	Ru1–P1	2.397(2)	2.48495
Ru1–P2	2.3592(11)	2.44167	Ru1–P2	2.376(18)	2.48840
N1–C7	1.335(7)	1.33992	N1–C7	1.351(9)	1.34448
N2–C7	1.321(5)	1.32063	N2–C7	1.261(10)	1.32807
N2–N3	1.404(5)	1.36885	N2–N3	1.388(8)	1.36536
N3–C8	1.296(5)	1.30713	N3– C8	1.284(9)	1.29941
C8–C9	1.463(6)	1.45541	C8–C9	1.442(10)	1.44495
C1–C6	1.414(6)	1.41257	C10–C11	1.386(10)	1.38973
C25–O1	1.168(5)	1.15876	C25–O1	1.143(9)	1.15630
N1–Ru1–N3	74.87(13)	73.94033	N1–Ru1–N3	75.20(2)	73.9149
C25−Ru1−N3	103.71(17)	104.57533	N3–Ru1–C10	78.60(3)	78.4514
C25−Ru1−H1	91.00(14)	88.63697	C10–Ru1–C25	103.90(3)	101.791
N1–Ru1–C25	178.19(16)	178.50026	N1–Ru1–C25	102.40(3)	105.841
P1–Ru1–P2	173.41(4)	172.67860	P1–Ru1–P2	176.91(7)	176.544

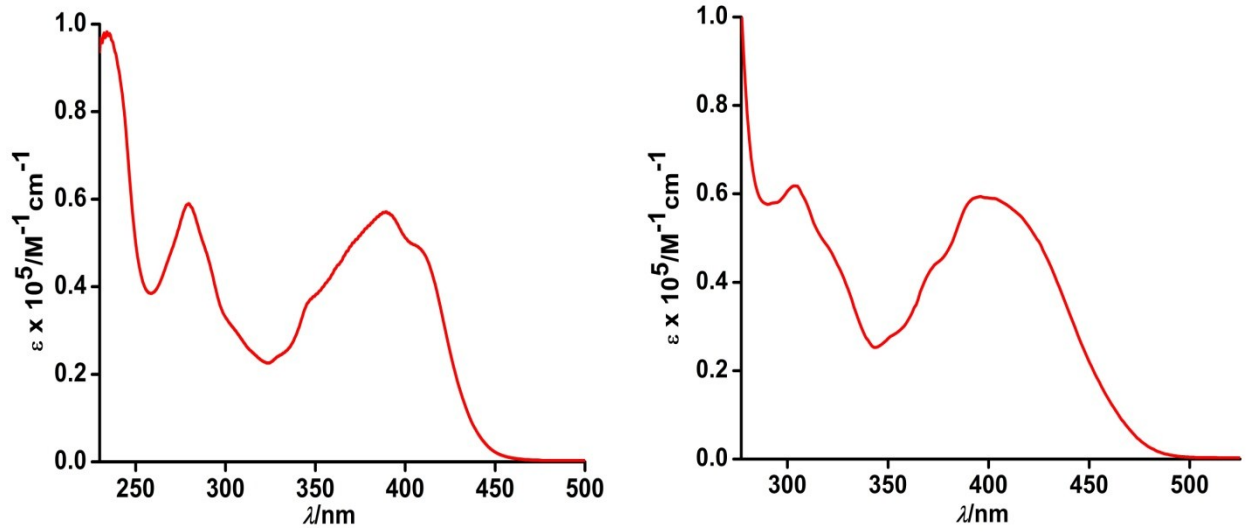


Fig. S1 Absorption spectra of **1a**(left) and **1b**(right) in dichloromethane at 298 K.

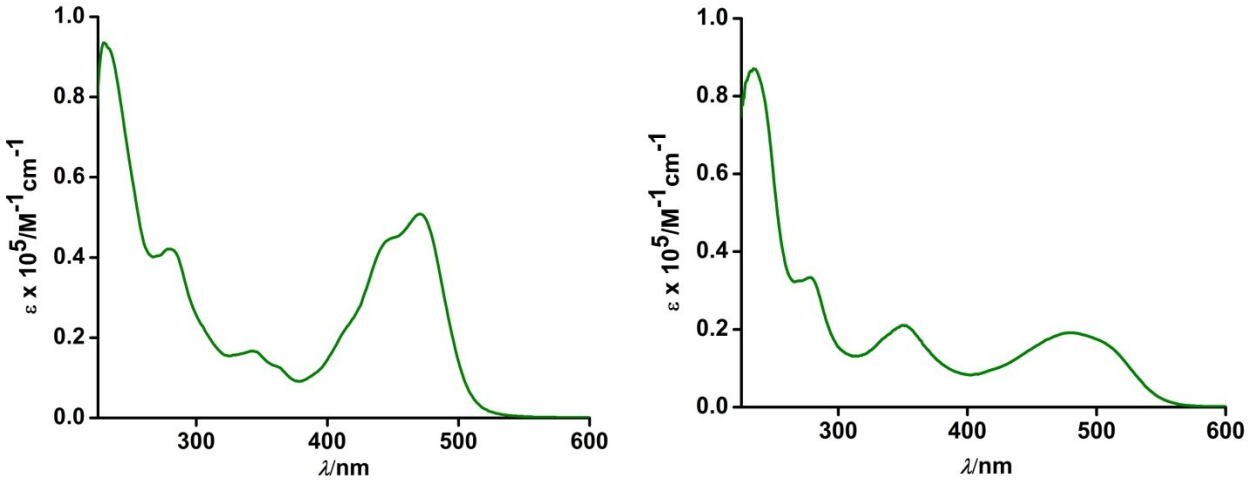


Fig. S2 Absorption spectra of **2a**(left) and **4a**(right) in dichloromethane at 298 K.

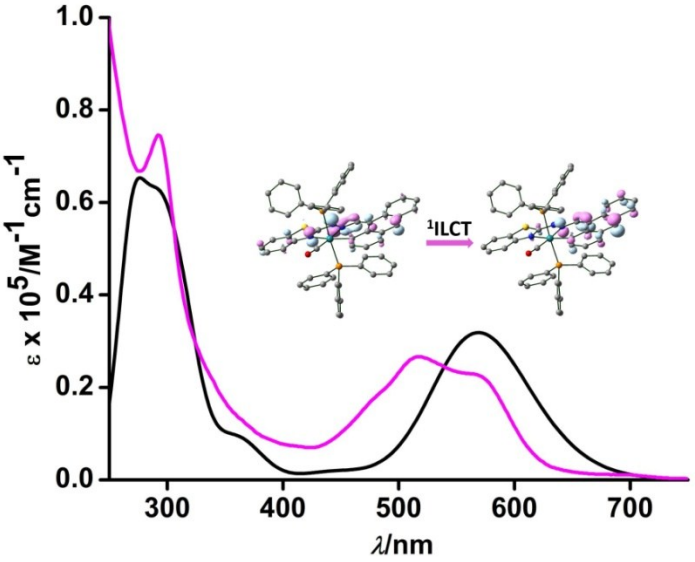


Fig. S3 Theoretical (black) and Experimental (magenta) electronic spectra of complexes **3b**

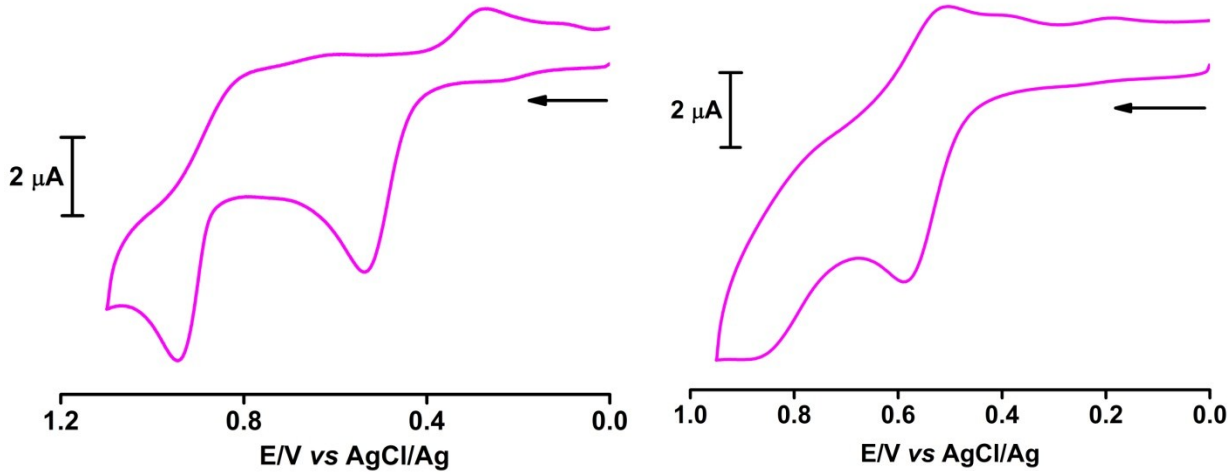


Fig. S4 Cyclic voltammogram of **3a** (left) and **5a** (right) in dichloromethane at 50 mVs^{-1}.

Table S5 Electrochemical data for complexes **3a**, **3b** and **5a**

Compounds	**$E_{1/2}$(ΔE/mV)**	**E_{pa}**
3a		+0.54, +0.95
3b	+0.53 (105)	+1.15
5a		+0.58, +0.86

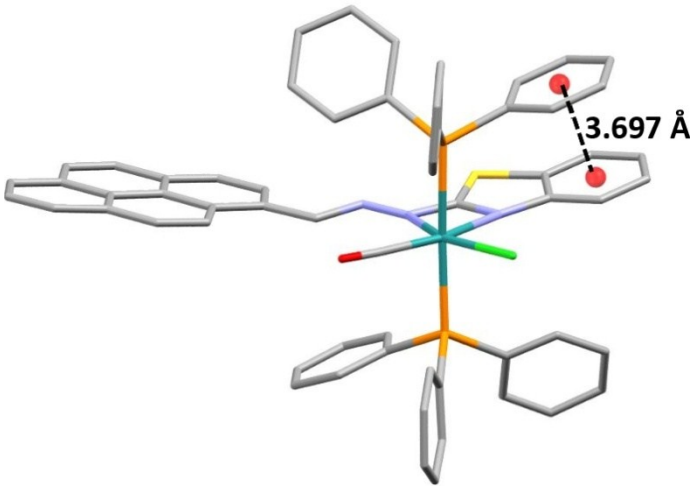


Fig. S5 π–π stacking interaction in complex **2a**(H atoms are omitted for clarity)

Table S6 Intramolecular π–π stacking parameters for compound **2a**

Stacking parameters	**phenyl-phenyl**
$d(c_i–c_j)$ Å/$\alpha°$	3.697(3)/ 8.3(2)
$d(\perp c_i–P_j)$ Å/$\beta°$	3.278(2)/27.6
$d(\perp c_j–P_i)$ Å/$\beta°$	3.295(2)/27.0

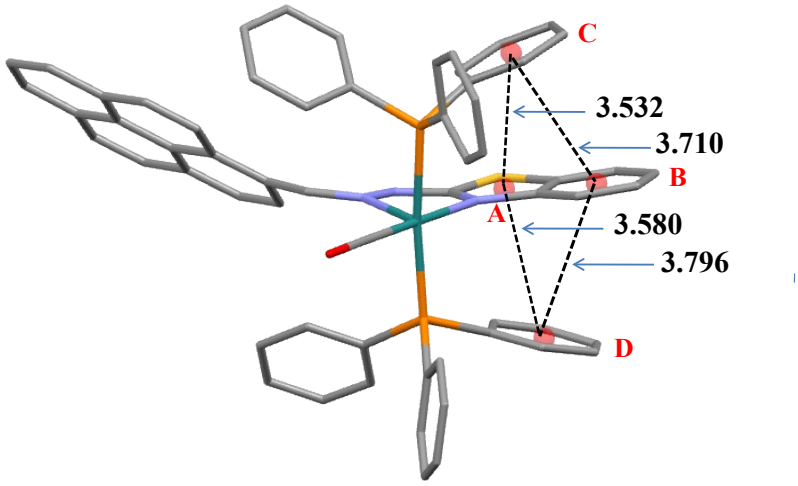


Fig. S6 π–π stacking interaction in complex **4a**(H atoms are omitted for clarity)

Table S7 Intramolecular π–π stacking parameters for compound **4a**

Stacking parameters	Rings			
	A−C	**A−D**	**B−C**	**B−D**
$d(c_i–c_j)$ Å/α °	3.532(4)/ 19.6(4)	3.580(4)/ 16.5(3)	3.710(5)/ 17.1(4)	3.797(4)/ 19.0(4)
$d(\perp c_i–P_j)$ Å/β °	3.363(3)/ 17.80	3.407(3)/ 17.90	3.370(3)/ 24.7	3.397(3)/ 26.5
$d(\perp c_j–P_i)$ Å/β' °	3.051(3)/ 30.30	3.135(3)/ 28.9	3.677(3)/ 7.6	3.763(3)/ 7.7

[a]c = ring centroid, α = dihedral angle between rings, β and β' (slip angle) = angle between the vector $c_i–c_j$ and the normal to plane P_i or P_j from c_i and c_j respectively, $d(c_i–c_j)$ = centroid-centroid distance, $d(\perp c_i–P_j)$ = ⊥ distance from c_i of P_i on ring P_i.

Ground State Geometries and Frontier Molecular Orbital Compositions

The FMOs are useful in elucidating the electronic structure, the electron transfer, and the optoelectronic properties of the synthesized complexes. All the C–H activated complexes are diamagnetic(t_2^6) at room temperature signifying their singlet ground state. The geometry optimizations of the complexes were performed using their crystallographic coordinates at (R)B3LYP levels in solvent phase in their singlet spin state without any ligand simplification. The optimized geometries of the synthesized complexes and the significant metrical parameters are given in ESI† (Fig. S18, S19 and Table S3, S4). The optimized structural parameters of **3a**, **3b** and **5a** are in general agreement with the experimental values with minor discrepancy that arises due to the crystal lattice distortion existing in actual molecules. The calculated Ru–C(PAH) distance is longer than the Ru–C(carbonyl) by approximately 0.25 Å. Isodensity plots of some selected FMOs of the Ru(II) complexes and energy levels (H − 1 to L + 2) are depicted in Fig. S9. The partial frontier molecular orbital compositions of the complexes along with the HOMO−LUMO energy gap, are listed Table S8, S11 and S14. In the ground state, the HOMO of the complexes have very high contribution of the ligand character while the more stabilized HOMO – 1 in both the complexes have substantial metal participation (~25%), along with reasonably high ligand character. The LUMO and LUMO + 1 are essentially of ligand character, the former having very high contribution from the PAH side while the latter has high contribution from the co-ligands.

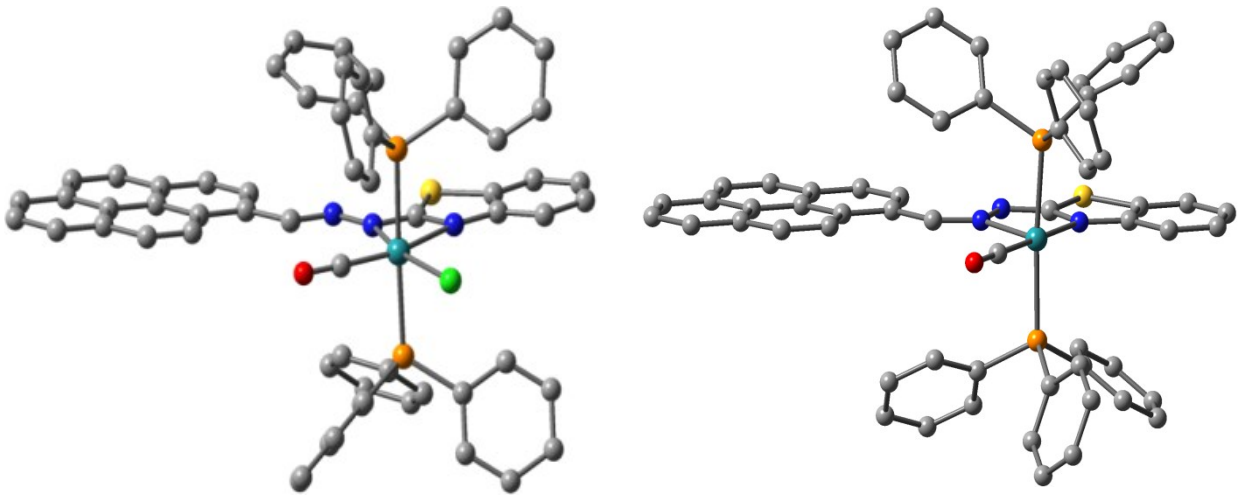


Fig. S7 Gas phase optimized geometries of **2a**(left) and **4a**(right).

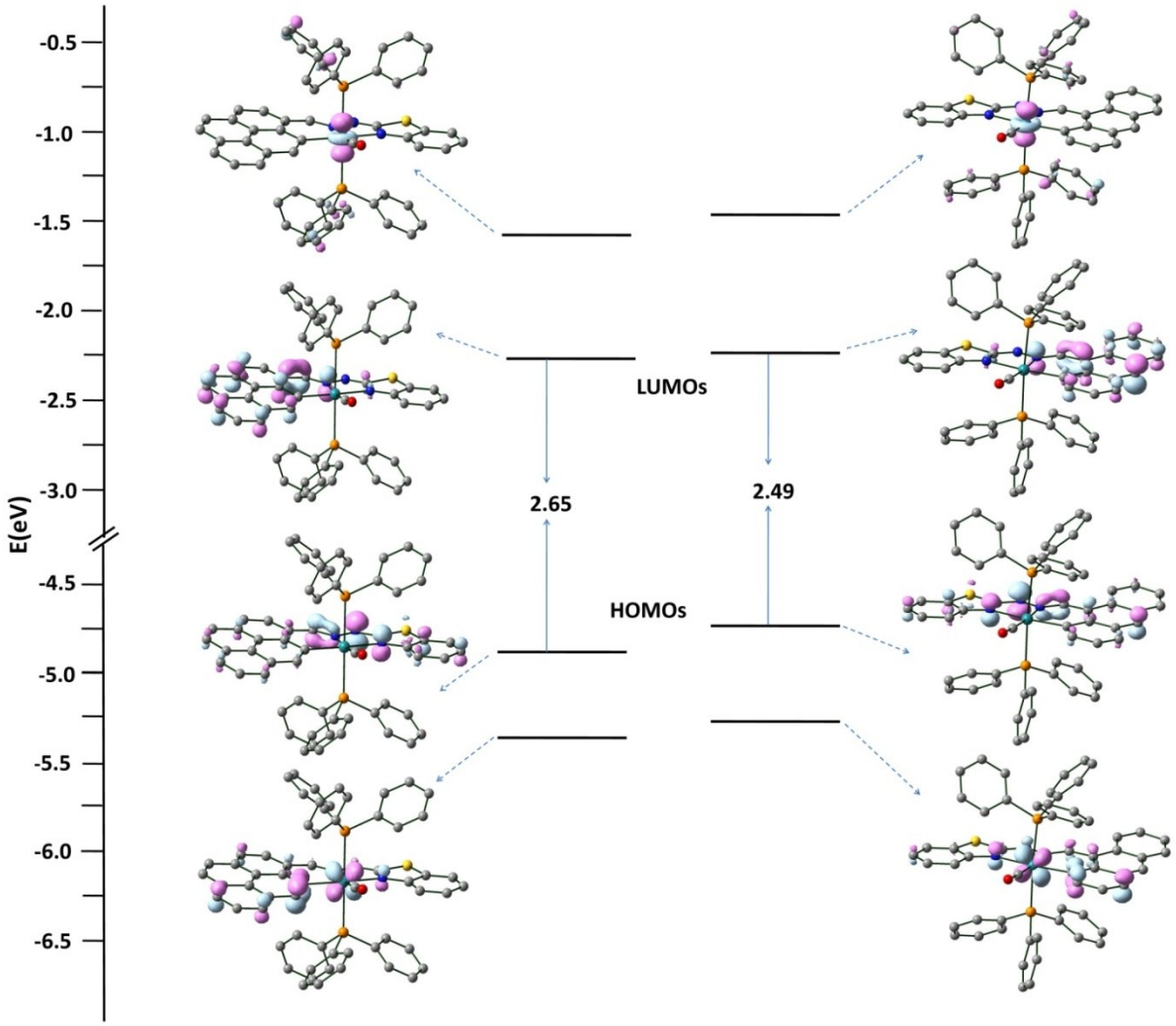


Fig. S8 A portion of MO diagram for complex **3a**(left) and **3b**(right)**.**

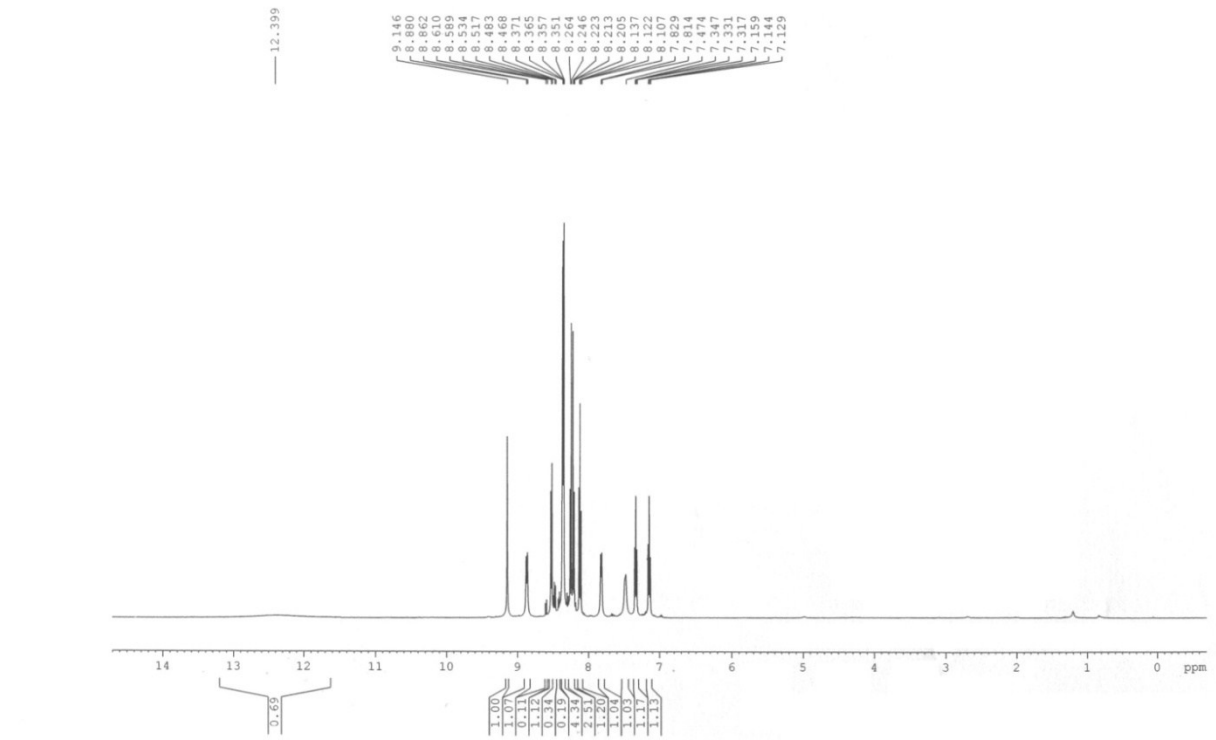


Fig. S9 ^{1}H-NMR spectrum of **1a**.

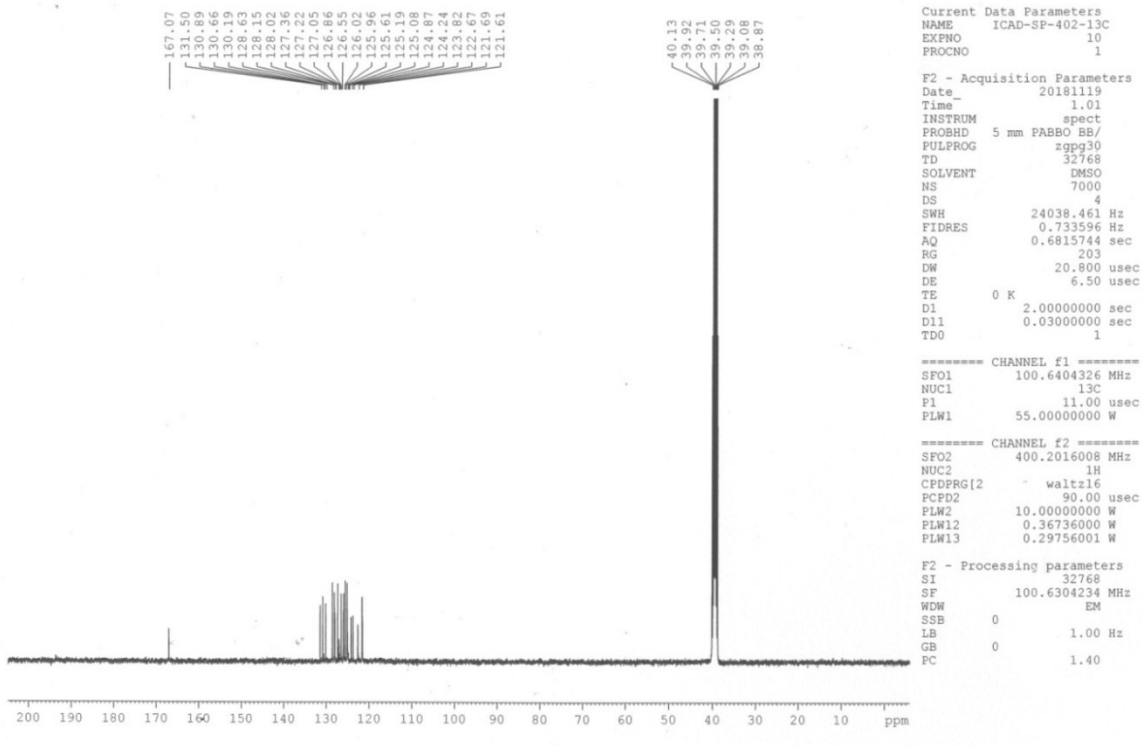


Fig. S10 ^{13}C-NMR spectrum of **1a**.

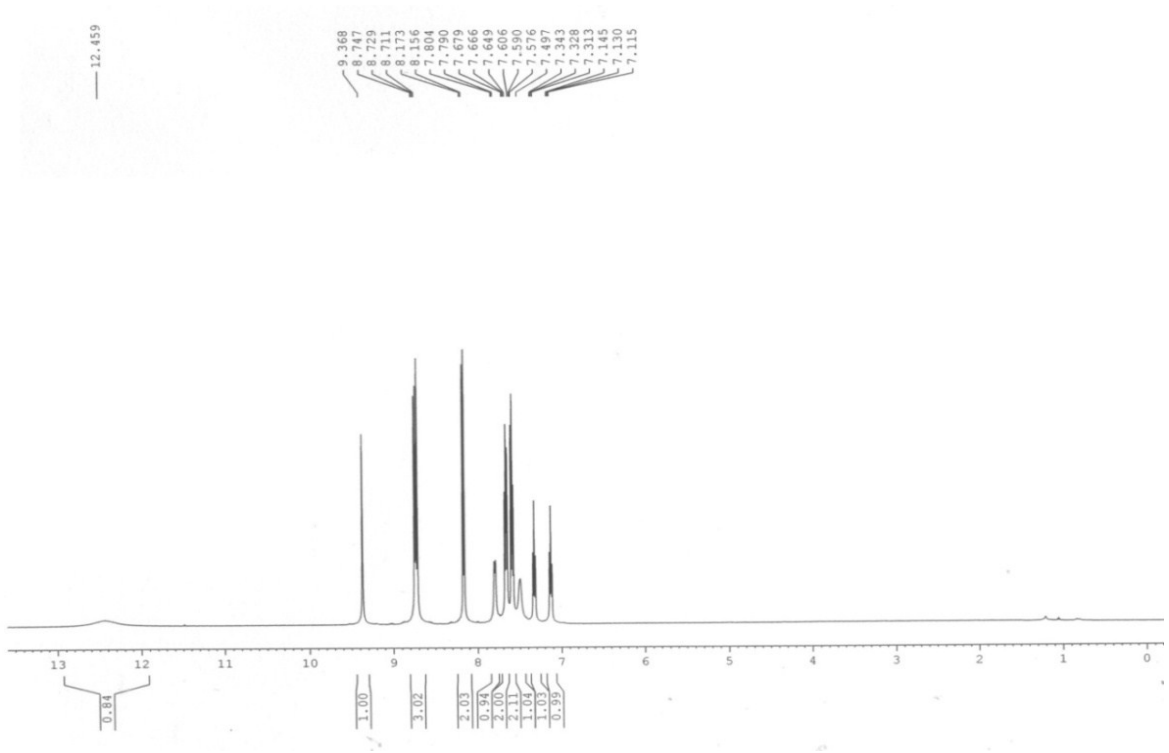


Fig. S11 [1]H-NMR spectrum of **1b**.

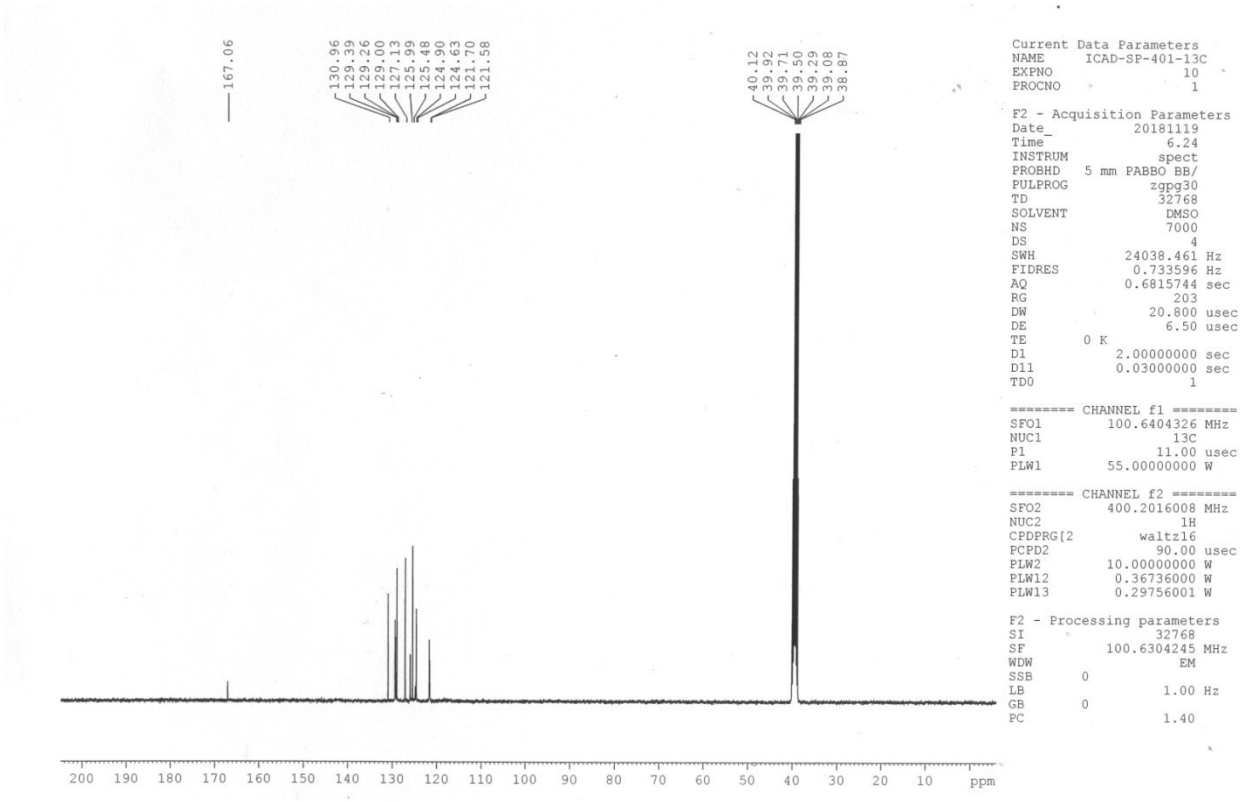


Fig. S12 [13]C-NMR spectrum of **1b**.

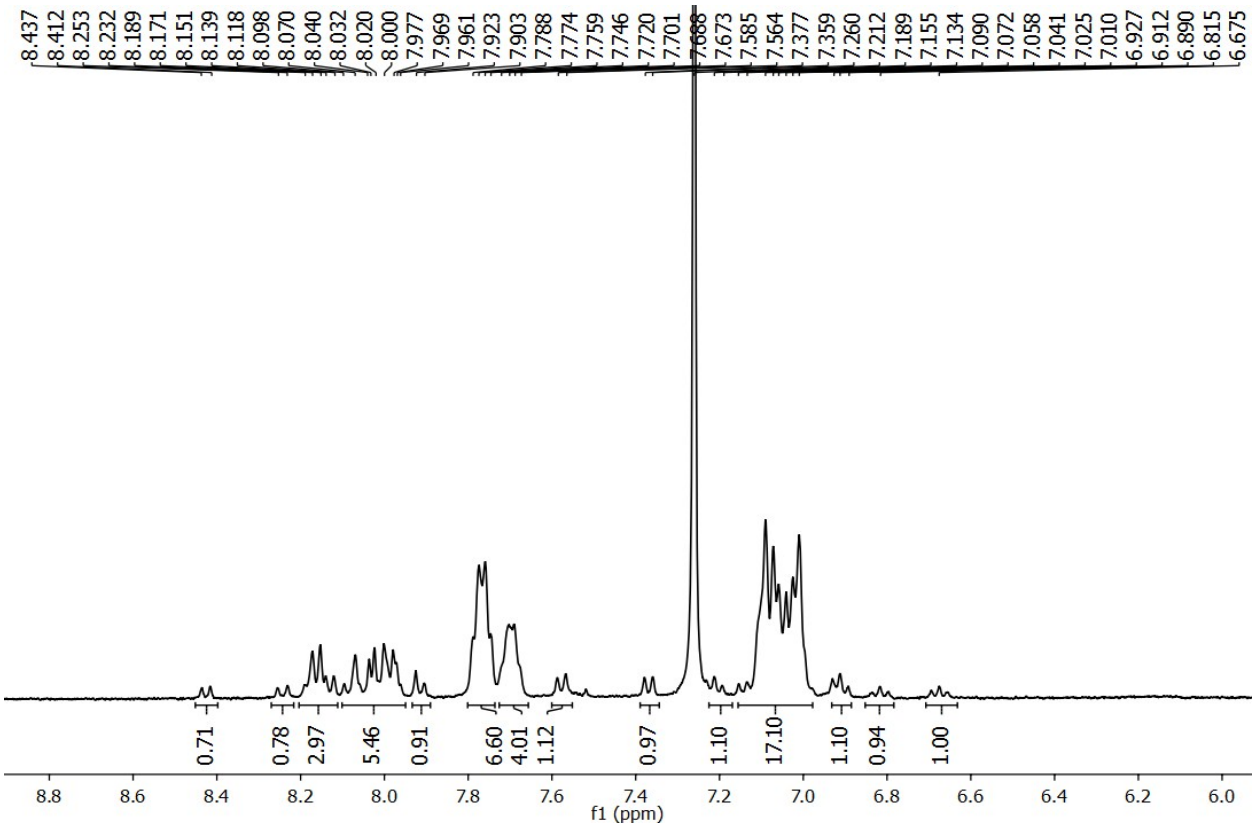


Fig. S13 [1]H-NMR spectrum of **2a**.

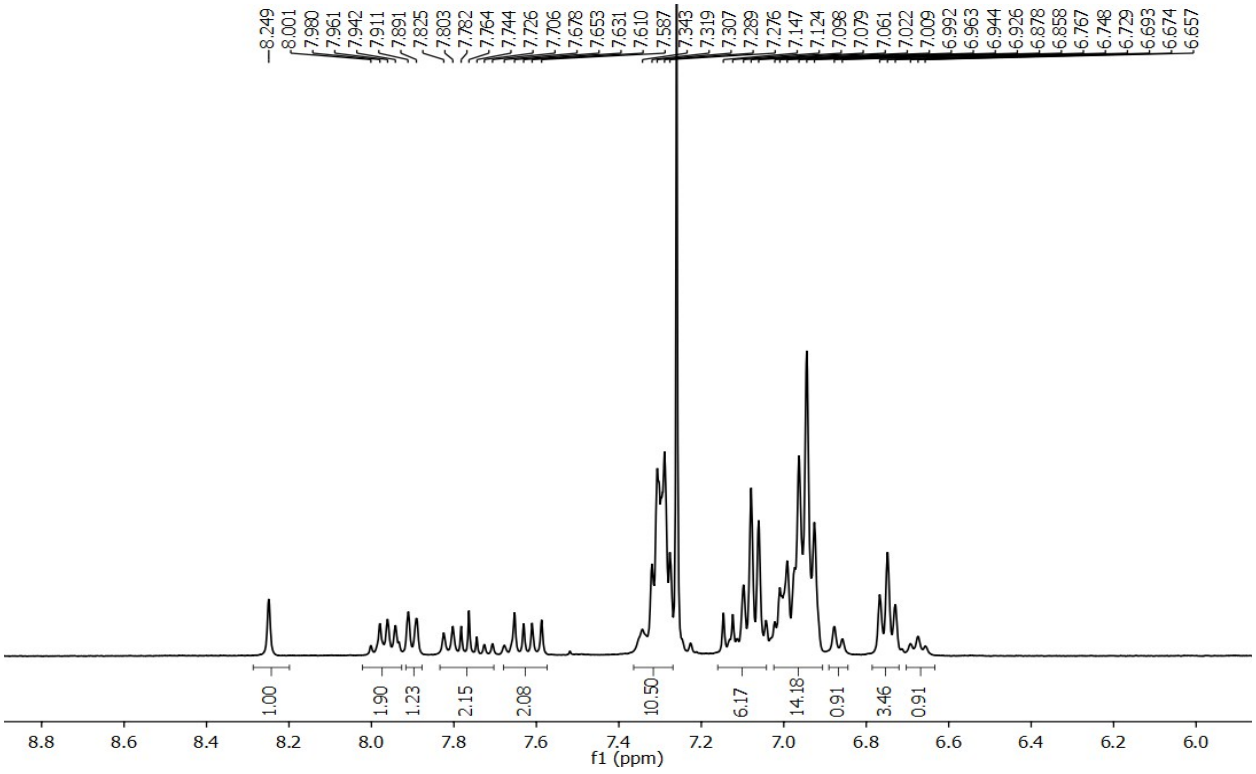


Fig. S14 [1]H-NMR spectrum of **3a**.

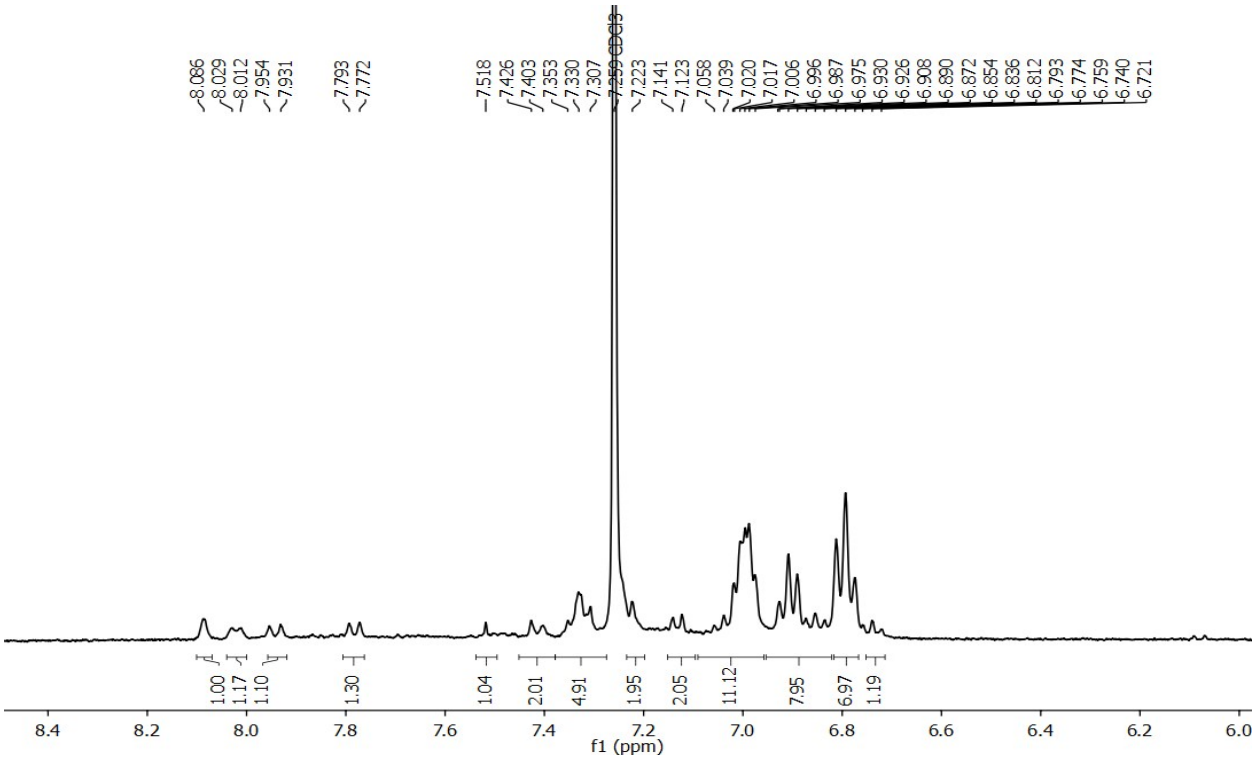


Fig. S15 [1]H-NMR spectrum of **3b**.

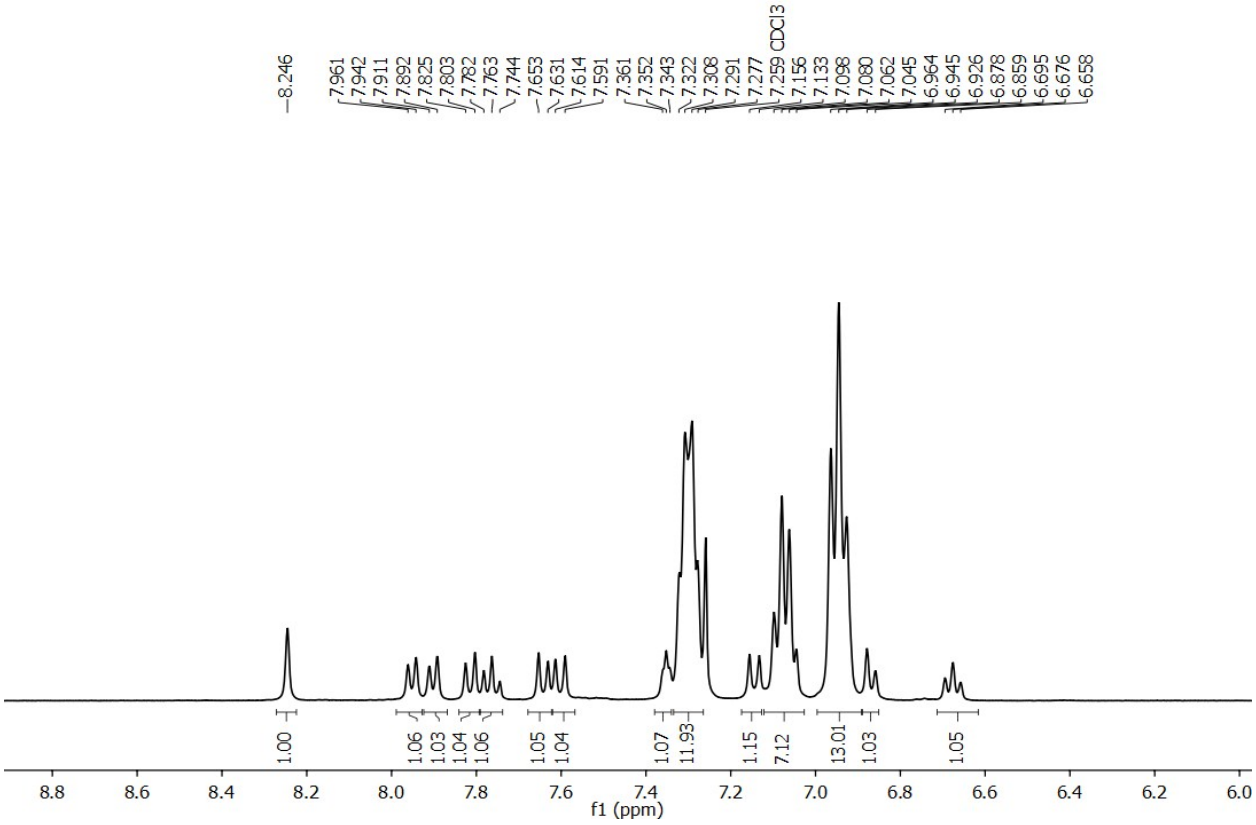


Fig. S16 [1]H-NMR spectrum of **5a**.

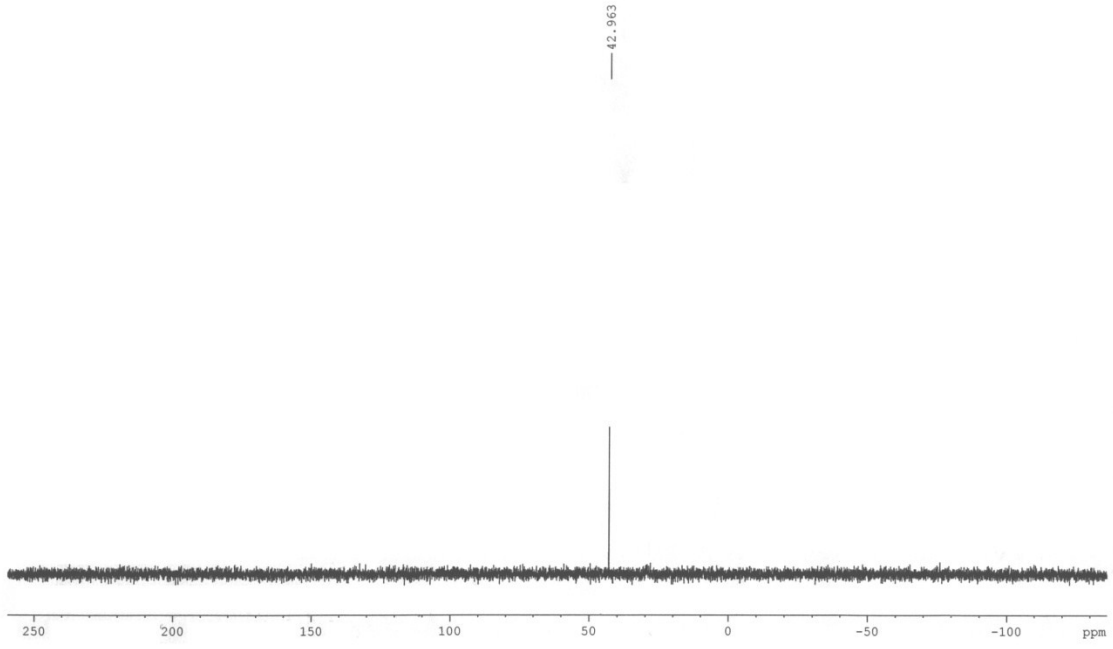


Fig. S17 ^{31}P-NMR spectrum of **2a**.

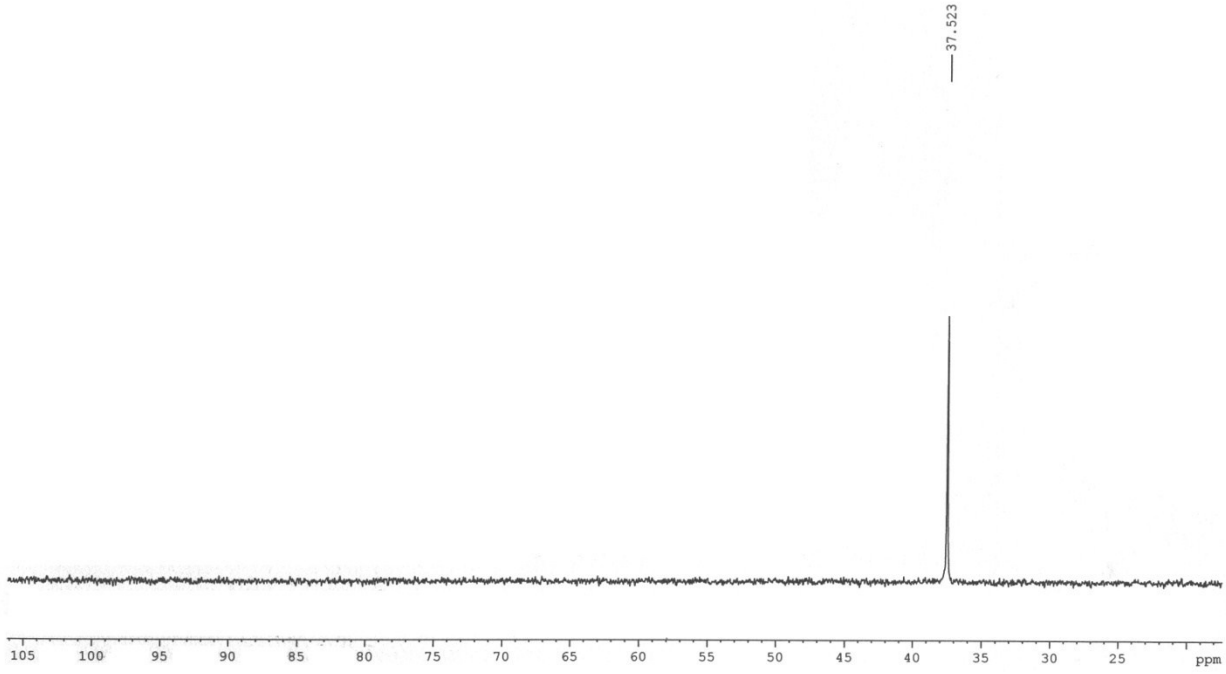


Fig. S18 ^{31}P-NMR spectrum of **3a**.

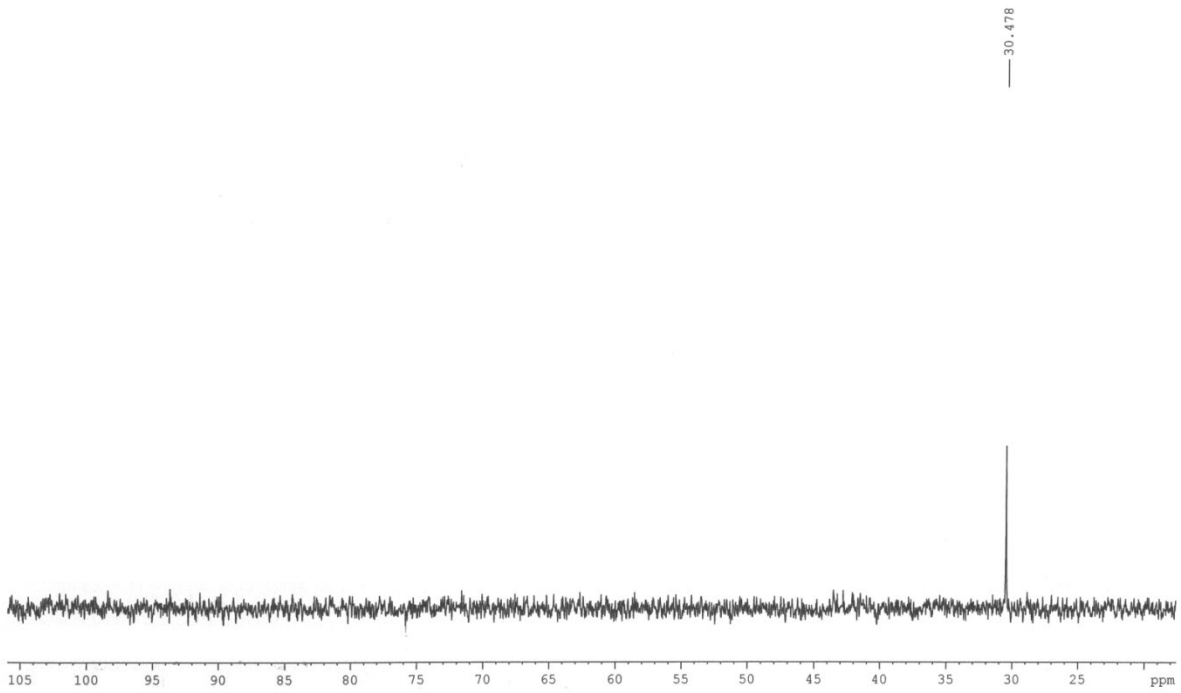


Fig. S19 ^{31}P-NMR spectrum of **3b**.

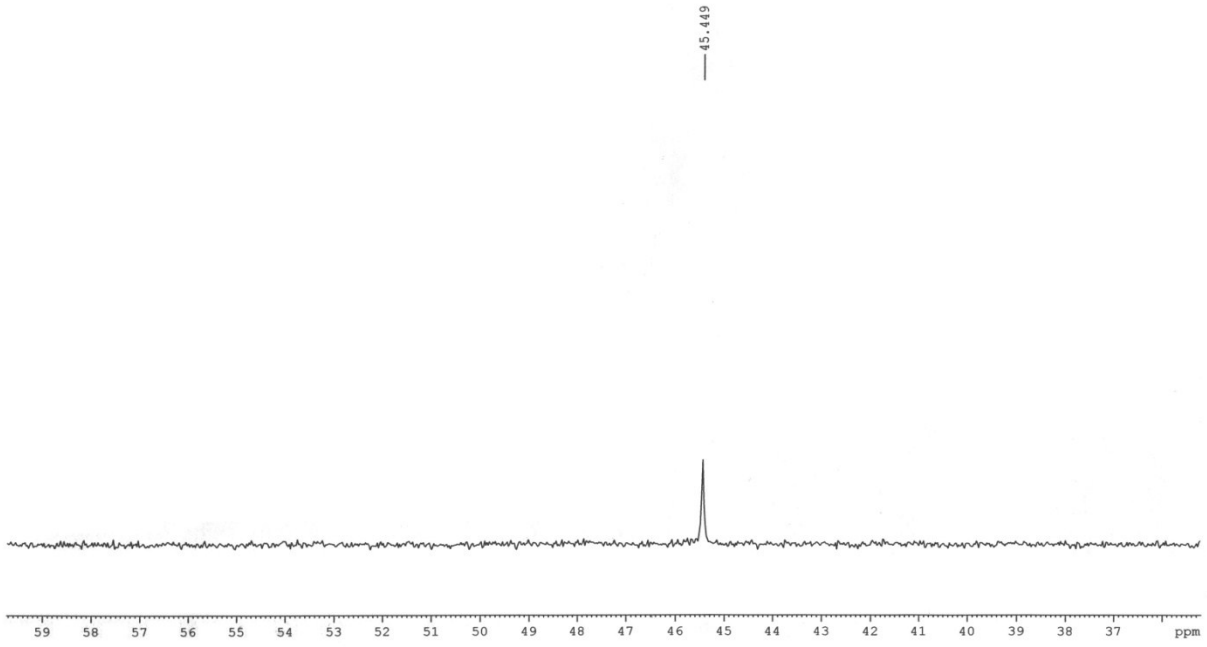


Fig. S20 ^{31}P-NMR spectrum of **4a**.

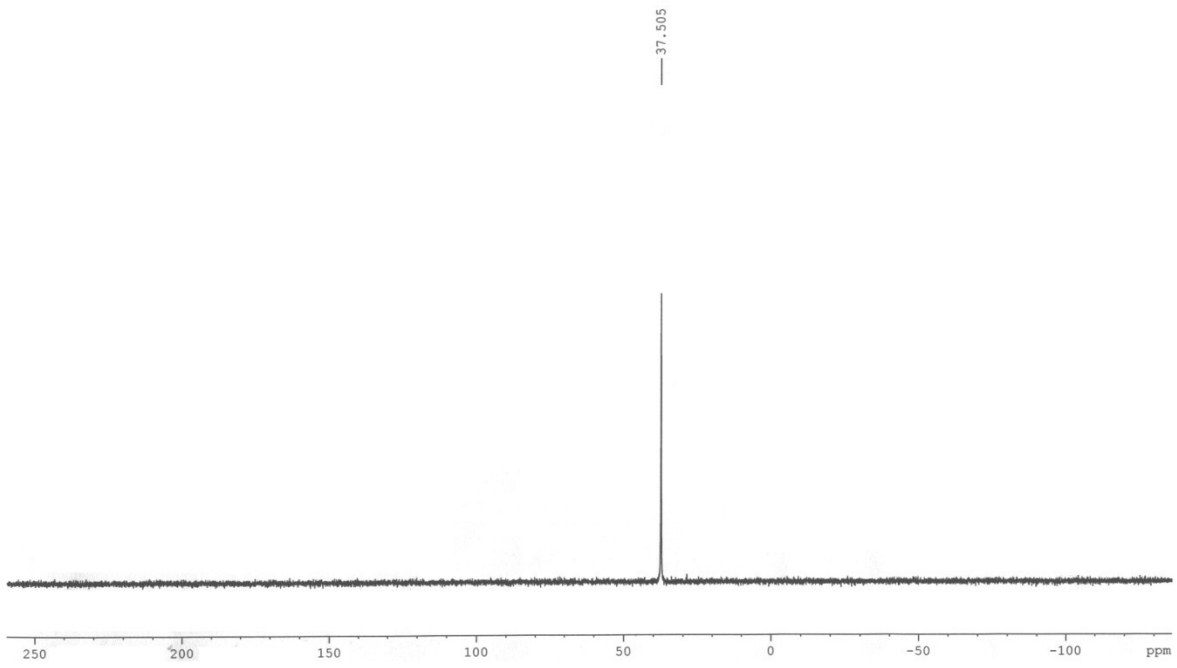


Fig. S21 ^{31}P-NMR spectrum of **5a**.

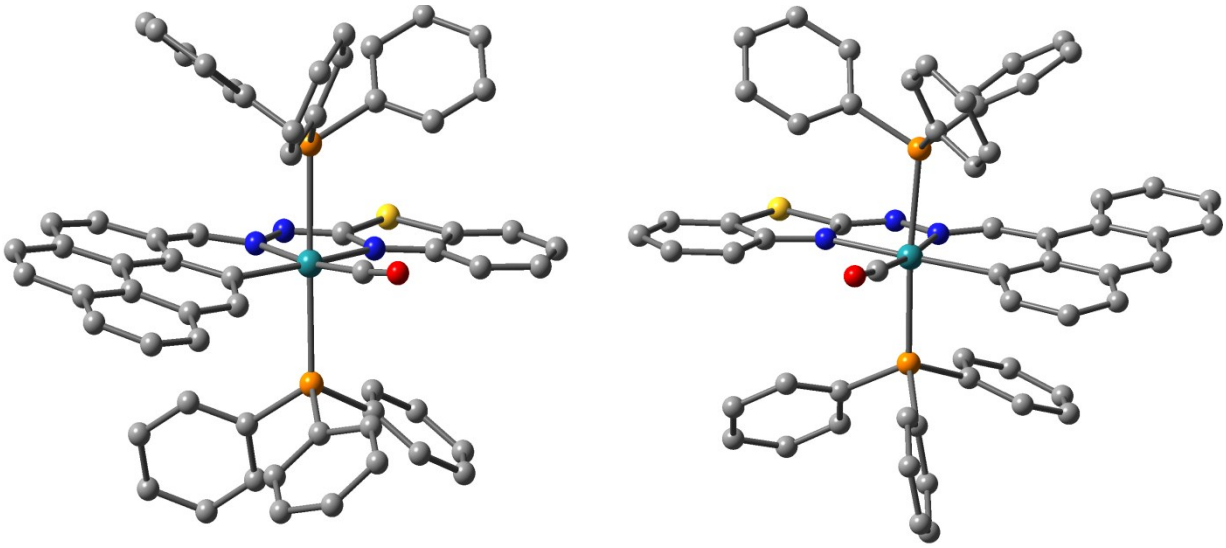


Fig. S22 Solution phase optimized geometries of **3a**(left) and **3b**(right).

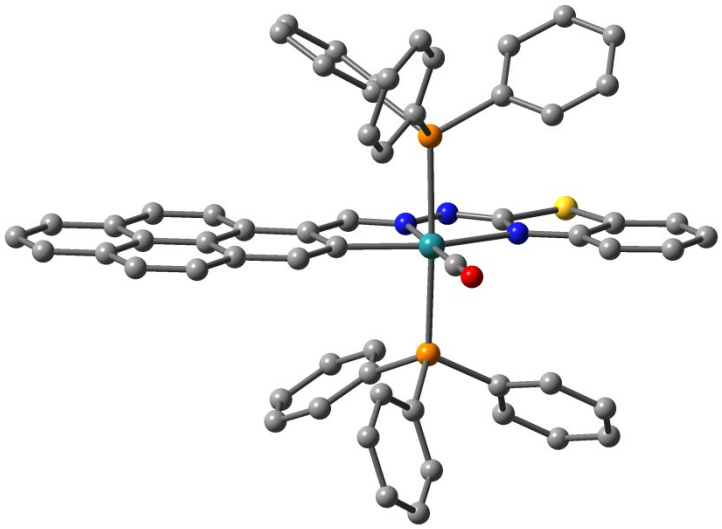


Fig. S23 Solution phase optimized geometries of **5a**

Table S8 Frontier molecular orbital composition (%) in the ground state for **3a**

Orbital	MO	Energy (EV)	Contribution (%)						Main Bond Type
			Metal	Ligand					
			Ru	Pyr	Hydrazone	Benz	PPh_3	CO	
256	L+5	-1.06	8	16	2	6	70	-2	$\pi^*(PPh_3)$
255	L+4	-1.11	1	45	2	2	49	0	$\pi^*(Pyr+PPh_3)$
254	L+3	-1.16	1	27	2	0	70	0	$\pi^*(PPh_3)$
253	L+2	-1.2	2	1	2	0	93	3	$\pi^*(PPh_3)$
252	L+1	-1.59	20	4	0	4	64	7	$Ru+\pi^*(PPh_3)$
251	LUMO	-2.3	1	68	20	8	1	1	π*(Pyr+Hydrazone)
250	HOMO	-5	2	32	28	35	2	0	π(Pyr+ Hydrazone+Benz)
249	H–1	-5.44	27	50	6	13	3	0	Ru +π(Pyr+Benz)
248	H–2	-6.24	21	42	3	31	3	0	Ru +π(Pyr+Benz)
247	H–3	-6.43	4	40	1	34	20	2	$\pi(Pyr+Benz+PPh_3)$
246	H–4	-6.59	59	15	1	7	6	12	Ru +π(Pyr+Benz)
245	H–5	-6.62	10	53	3	26	8	1	$\pi(PPh_3+Pyr+CO)$
HOMO–LUMO gap = 2.70 eV									

Table S9 Main optical transition at the TD-DFT/B3LYP/6-311+G(d,p) Level for the complex **3a** with composition in terms of molecular orbital contribution of the transition, Computed Vertical excitation energies, and oscillator strength in dichloromethane

Transition	**CI**	**Composition**	**E (eV)**	**Oscillator strength (*f*)**	**λ_{theo} (nm)**
$S_0 \rightarrow S_1$	0.68892	HOMO → LUMO (95%)	2.2906	0.4925	541.28
$S_0 \rightarrow S_2$	0.67023	H–1 → LUMO (90%)	2.6220	0.1615	472.85
$S_0 \rightarrow S_{24}$	0.45924	H–5 → LUMO (42%)	3.8716	0.0862	320.24
$S_0 \rightarrow S_{63}$	0.47539	H–6→ L+1 (45%)	4.5581	0.2044	272.01

Table S10 Natural transition orbitals (NTOs) for complex **3a** illustrating the nature of singlet excited states in the absorption bands in the range 200–700 nm. For each state, the respective number of the state, transition energy (eV), and the oscillator strength (in parentheses) are listed. Shown are only occupied (holes) and unoccupied (electrons) NTO pairs that contribute more than 10% to each excited state

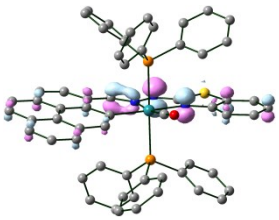
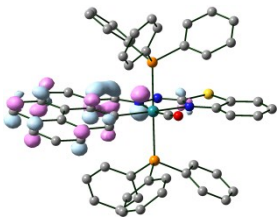
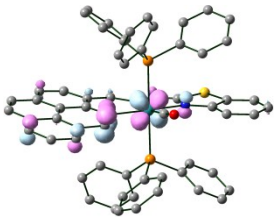
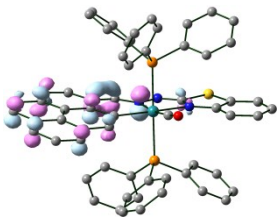
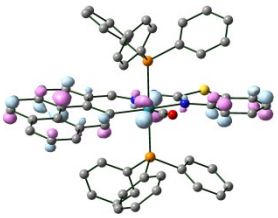
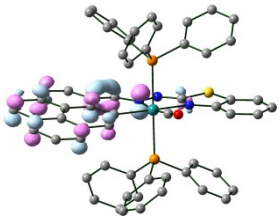
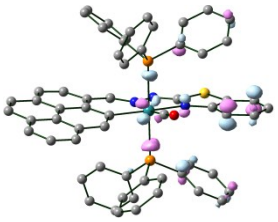
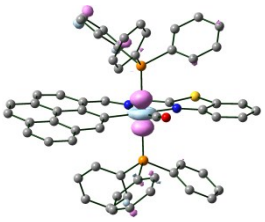
		Hole	Electron
545 nm	S_1 w = 0.9492 2.2906 (0.4925) 541.28 nm ILCT π(Hydrazone + Benz) → π*(Pyr +hydrazone)		
447 nm	S_2 w = 0.8984 2.6220 (0.1615) 472.85 nm ILCT +MLCT π (Pyr)+d_{xz}(Ru) → π*(Pyr + hydrazone)		
379 nm	S_{24} w = 0.4218 3.8716 (0.0951) 320.24 nm ILCT+MLCT π(Pyr+Benz)+d_{yz}(Ru)→ π*(Pyr + hydrazone)		
314 nm	S_{63} w = 0.4519 4.5581 (0.2044) 272.01 nm LLCT+ d-d transition π(Benz)+ d_{yz}(Ru)→ π*(PPh_3)+ d_z^2(Ru)		

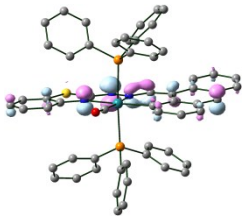
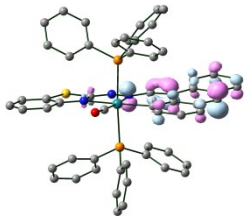
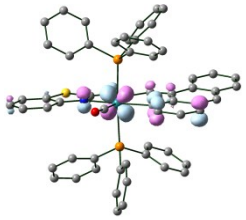
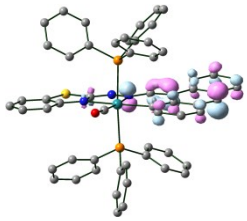
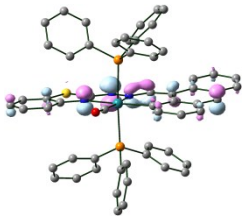
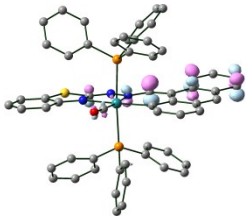
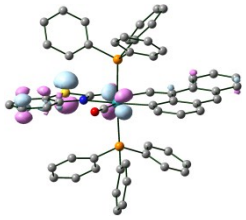
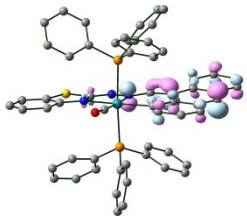
Table S11 Frontier molecular orbital composition (%) in the ground state for **3b**

Orbital	MO	Energy (EV)	Contribution (%)						Main Bond Type
			Metal	Ligand					
			Ru	Anc	Hydrazone	Benz	PPh_3	CO	
250	L+5	-1.03	4	14	10	6	66	1	$\pi^*(PPh_3)$
249	L+4	-1.07	11	5	0	3	84	-1	$\pi^*(PPh_3)$
248	L+3	-1.18	1	0	0	1	94	3	$\pi^*(PPh_3)$
247	L+2	-1.23	1	1	1	1	95	1	$\pi^*(PPh_3)$
246	L+1	-1.54	19	5	0	0	71	6	$Ru+\pi^*(PPh_3)$
245	LUMO	-2.37	1	73	18	8	0	1	π*(Anthracene+Hydrazone)
244	HOMO	-4.93	1	40	26	31	2	0	π(Anc+ Hydrazone+Benz)
243	H–1	-5.4	28	42	10	18	2	0	Ru +π(Anc+Benz)
242	H–2	-6.28	21	17	4	50	9	0	Ru +π(Anc+Benz)
241	H–3	-6.54	41	28	0	18	3	9	Ru +π(Anc+Benz)
240	H–4	-6.55	24	26	1	28	16	4	Ru +π(Anc+Benz+CO)
239	H–5	-6.69	5	40	0	20	35	0	$\pi(PPh_3$+Anc)
HOMO–LUMO gap = 2.56 eV									

Table S12 Main optical transition at the TD-DFT/B3LYP/6-311+G(d,p) Level for the complex **3b** with composition in terms of molecular orbital contribution of the transition, Computed Vertical excitation energies, and oscillator strength in dichloromethane

Transition	CI	Composition	E (eV)	Oscillator strength (*f*)	λ_{theo} (nm)
$S_0 \rightarrow S_1$	0.69545	HOMO → LUMO (97%)	2.1774	0.4321	569.41
$S_0 \rightarrow S_2$	0.68838	H–1 → LUMO (95%)	2.4477	0.0321	506.53
$S_0 \rightarrow S_{12}$	0.54342 0.01126	HOMO → L+7 (59%) H–2 → LUMO (13%)	3.4644	0.0732	357.88
$S_0 \rightarrow S_{57}$	0.50700	H–4→ L+1 (51%)	4.4150	0.1258	280.82

Table S13 Natural transition orbitals (NTOs) for complex **3b** illustrating the nature of singlet excited states in the absorption bands in the range 200–700 nm. For each state, the respective number of the state, transition energy (eV), and the oscillator strength (in parentheses) are listed. Shown are only occupied (holes) and unoccupied (electrons) NTO pairs that contribute more than 10% to each excited state

		Hole	Electron
566 nm	S_1 w = 0.9673 2.1774 (0.4321) 569.41 nm ILCT π(Hydrazone+Anc) → π*(Anc)		
515 nm	S_2 w = 0.9477 2.4477 (0.0321) 506.53 nm ILCT d_{yz} (Ru)+ π*(Anc) → π*(Anc)		
348 nm	S_{12} w = 0.4353 3.4644 (0.0732) 357.88 nm ILCT π(Hydrazone+Anc) → π* (Hydrazone+Anc)		
	S_{12} w = 0.0025 3.4366 (0.0732) 357.88nm ILCT/MLCT d_{yz} (Ru)+ π*(Anc) → π*(Hydrazone+Anc)		

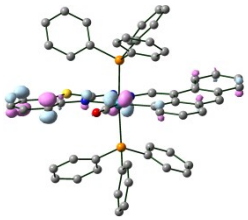
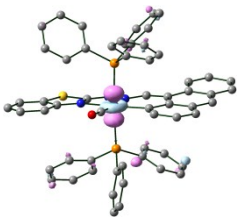
291 nm	S_{57} w = 0.5140 4.4150 (0.1258) 280.82 nm ILCT+LMCT π*(Benz)+ d_{xy} (Ru)→ d_z^2 (Ru)		

Table S14 Frontier molecular orbital composition (%) in the ground state for **5a**

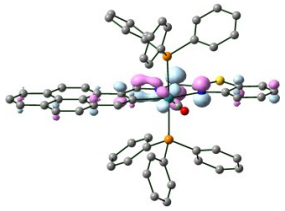
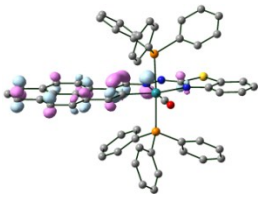
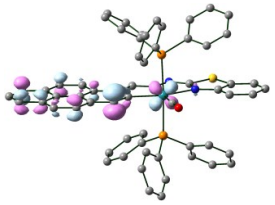
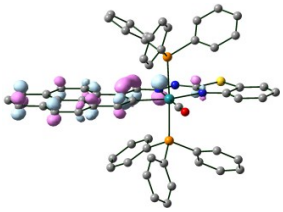
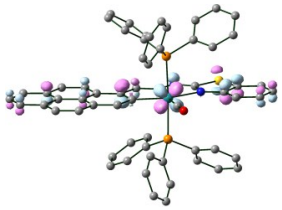
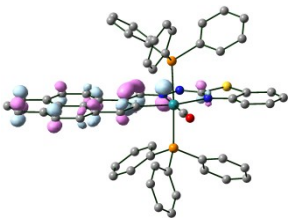
Orbital	MO	Energy (EV)	Contribution (%)						Main Bond Type
			Metal	Ligand					
			Ru	Pyr	Hydrazone	Benz	PPh_3	CO	
256	L+5	-0.91	2	45	18	5	27	3	π*(Hydrazone+Pyr+PPh_3)
255	L+4	-0.93	5	0	0	4	91	0	Ru+π*(PPh_3)
254	L+3	-1.09	0	3	1	1	93	2	π*(PPh_3)
253	L+2	-1.14	0	0	0	1	96	3	π*(PPh_3)
252	L+1	-1.33	16	1	1	0	76	6	d_z^2(Ru)+π*(PPh_3)
251	LUMO	-2.22	0	68	20	10	0	1	π*(Pyr+Hydrazone+Benz)
250	HOMO	-4.92	7	32	28	32	1	0	π(Pyr+ Hydrazone+Benz)
249	H–1	-5.46	22	71	1	5	1	0	d_{yz}(Ru)+π(Pyr)
248	H–2	-5.89	19	40	8	31	2	0	d_{yz}(Ru)+π(Pyr+Benz)
247	H–3	-6.18	2	15	1	69	13	0	π(Anc+Benz)
246	H–4	-6.20	49	31	0	9	0	13	d_{xy}(Ru)+π(Pyr+CO)
245	H–5	-6.54	6	4	1	19	68	2	π(Pyr+PPh_3)
HOMO–LUMO gap = 2.70 eV									

Table S15 Main optical transition at the TD-DFT/B3LYP/6-311+G(d,p) Level for the complex **5a** with composition in terms of molecular orbital contribution of the transition, Computed Vertical excitation energies, and oscillator strength in dichloromethane

Transition	CI	Composition	E (eV)	Oscillator strength (*f*)	λ_{theo} (nm)
$S_0 \rightarrow S_1$	0.69036	HOMO → LUMO (95%)	2.2252	0.5695	557.18
$S_0 \rightarrow S_3$	0.61247	H–1 → LUMO (75%)	2.9734	0.3282	416.98

$S_0 \rightarrow S_{17}$	0.46658	H–2 $\rightarrow$ LUMO (69%)	3.7286	0.0236	332.52
$S_0 \rightarrow S_{75}$	0.47509	H–3$\rightarrow$ L+3 (45%)	4.7073	0.0278	263.39

Table S16 Natural transition orbitals (NTOs) for complex **5a** illustrating the nature of singlet excited states in the absorption bands in the range 200–700 nm. For each state, the respective number of the state, transition energy (eV), and the oscillator strength (in parentheses) are listed. Shown are only occupied (holes) and unoccupied (electrons) NTO pairs that contribute more than 10% to each excited state

		Hole	Electron
567 nm	S_1 w = 0.9531 2.2252 (0.5695) 557.18 nm ILCT+MLCT π(Hydrazone)+ d_{yz} (Ru)→ π*(Pyr+Hydrazone)		
380 nm	S_3 w = 0.7502 2.9734 (0.3282) 416.98 nm ILCT+MLCT π*(Pyr) + d_{yz} (Ru) → π*(Pyr)		
318 nm	S_{17} w = 0.4353 3.7286 (0.0236) 332.52 nm ILCT+MLCT π(Hydrazone+Pyr) + d_{yz}(Ru) → π* (Hydrazone+Anc)		

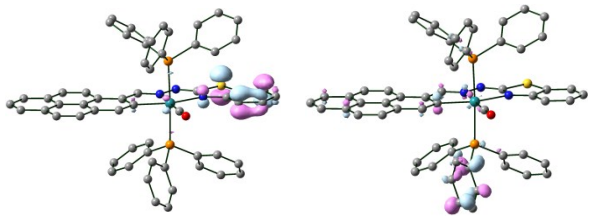
234 nm	S_{75} w = 0.4514 4.7073(0.0278) 263.39 nm LLCT π*(Benz) → π*(PPh_3)	

Table S17 Gas phase optimized coordinates of **2a**

Tag	Symbol	X	Y	Z
1	Ru	12.92007	6.988955	13.34261
2	Cl	13.44731	5.022292	14.75905
3	N	10.79841	7.651322	14.0562
4	C	9.590751	7.64032	14.73394
5	C	9.161044	6.687795	15.66948
6	H	9.798652	5.843111	15.90933
7	C	7.906935	6.833744	16.26324
8	H	7.571847	6.09353	16.98528
9	C	7.070703	7.912557	15.93835
10	H	6.097707	8.00849	16.41207
11	C	7.479307	8.865752	14.99975
12	H	6.832025	9.698955	14.73954
13	C	8.73107	8.72107	14.40457
14	S	9.477408	9.761145	13.17871
15	C	10.87337	8.677326	13.20897
16	N	11.99183	8.727736	12.48332
17	N	12.09983	9.69767	11.56149
18	C	13.1583	9.716276	10.81482
19	H	13.91283	8.943675	10.95025
20	C	13.35771	10.74154	9.796354
21	C	12.39742	11.7642	9.640256
22	H	11.53196	11.75693	10.2947
23	C	12.53765	12.754	8.683174
24	H	11.77869	13.52802	8.589614
25	C	13.65156	12.77875	7.820918
26	C	13.81462	13.79345	6.820153
27	H	13.04857	14.56128	6.735354
28	C	14.89794	13.80537	5.990122
29	H	15.00655	14.58206	5.236385
30	C	15.91755	12.79879	6.090185
31	C	17.04321	12.78993	5.245868

32	H	17.14531	13.56892	4.493552
33	C	18.01968	11.80083	5.365228
34	H	18.88255	11.81084	4.704175
35	C	17.89534	10.79922	6.329105
36	H	18.65938	10.03039	6.419639
37	C	16.78719	10.76847	7.193878
38	C	16.62442	9.75645	8.197959
39	H	17.38967	8.988995	8.290973
40	C	15.54212	9.738984	9.028547
41	H	15.47697	8.948449	9.767126
42	C	14.50368	10.73451	8.947048
43	C	14.64461	11.76007	7.952792
44	C	15.78018	11.77542	7.081507
45	P	11.86065	5.540118	11.63708
46	C	12.90614	4.196561	10.89794
47	C	14.07592	3.760733	11.53548
48	H	14.38619	4.212443	12.47024
49	C	14.82827	2.711994	10.99471
50	H	15.73194	2.387299	11.50398
51	C	14.42082	2.084849	9.816886
52	H	15.00793	1.271627	9.397494
53	C	13.24642	2.503521	9.181342
54	H	12.91482	2.017252	8.26726
55	C	12.49323	3.54659	9.719957
56	H	11.58434	3.856646	9.2133
57	C	10.3574	4.579315	12.14169
58	C	10.30697	4.038583	13.43594
59	H	11.10697	4.24712	14.13926
60	C	9.24733	3.209497	13.81383
61	H	9.227282	2.793778	14.81824
62	C	8.221172	2.917054	12.91284
63	H	7.395117	2.276563	13.21165
64	C	8.265112	3.450544	11.62178
65	H	7.47456	3.227481	10.90946
66	C	9.328258	4.270035	11.23556
67	H	9.34612	4.665887	10.22549
68	C	11.32329	6.523707	10.16897
69	C	12.19114	6.710442	9.079605
70	H	13.15427	6.209184	9.055634
71	C	11.82574	7.531194	8.009531
72	H	12.51082	7.660968	7.175802
73	C	10.59284	8.187538	8.01587
74	H	10.31108	8.829349	7.185309
75	C	9.730478	8.024141	9.103277
76	H	8.774871	8.541484	9.127407
77	C	10.09373	7.203094	10.1728

78	H	9.411456	7.095448	11.01061
79	P	13.99558	8.355729	15.13868
80	C	15.84603	8.323726	15.06254
81	C	16.47467	7.066214	15.0119
82	H	15.87265	6.161424	14.99862
83	C	17.86689	6.973245	14.98908
84	H	18.33669	5.993683	14.95107
85	C	18.65274	8.130152	15.00819
86	H	19.73703	8.055556	14.98365
87	C	18.036	9.381753	15.05999
88	H	18.63634	10.28798	15.07933
89	C	16.64063	9.479706	15.09262
90	H	16.18162	10.46107	15.14637
91	C	13.55749	10.15163	15.14216
92	C	13.87125	10.93822	14.0213
93	H	14.38131	10.49638	13.17126
94	C	13.53325	12.29105	13.98003
95	H	13.78549	12.8794	13.10176
96	C	12.86152	12.8786	15.05667
97	H	12.59126	13.93098	15.02288
98	C	12.53409	12.10402	16.17148
99	H	12.00741	12.5494	17.01174
100	C	12.88017	10.74973	16.21677
101	H	12.62173	10.16518	17.09335
102	C	13.67042	7.843552	16.88431
103	C	12.42414	7.305992	17.23116
104	H	11.68061	7.139712	16.46348
105	C	12.13593	6.980594	18.55845
106	H	11.16251	6.567157	18.8093
107	C	13.09677	7.1759	19.55399
108	H	12.87599	6.914504	20.58592
109	C	14.34589	7.704055	19.21543
110	H	15.10194	7.855918	19.98174
111	C	14.63172	8.038359	17.88919
112	H	15.60598	8.448265	17.64306
113	C	14.50394	6.921027	12.40923
114	O	15.48559	6.90625	11.78614

Table S18 Gas phase optimized coordinates of **3a**

Tag	Symbol	X	Y	Z
1	Ru	6.749503	5.120425	6.028174
2	P	6.84595	3.486793	4.101712
3	P	6.629157	6.717357	7.97078
4	S	10.76981	3.587734	7.766059
5	N	8.236808	3.894552	7.129596
6	N	9.747794	5.442166	6.120491
7	N	8.616135	5.990124	5.552941
8	O	4.202873	3.915176	7.162322
9	C	4.951929	7.292947	8.528478
10	C	4.225834	8.388974	3.168492
11	C	9.044822	1.89988	4.777832
12	H	9.582518	2.843212	4.769146
13	C	7.553645	8.315597	7.807151
14	C	7.741867	3.932463	2.532448
15	C	7.668101	1.868426	4.492317
16	C	7.265723	5.992645	9.559321
17	C	8.956806	8.316967	7.701543
18	H	9.510548	7.382555	7.697471
19	C	6.400176	7.672154	4.175098
20	C	8.354333	2.94164	1.742835
21	H	8.352599	1.906042	2.064421
22	C	5.759326	6.484451	4.74407
23	C	5.16226	4.362525	6.67593
24	C	8.291454	2.779952	7.95125
25	C	5.17042	3.008075	3.459784
26	C	8.276874	6.572222	10.34028
27	H	8.773206	7.479165	10.01548
28	C	9.454334	4.41522	6.902832
29	C	3.900883	7.434993	7.612018
30	H	4.050954	7.173742	6.572396
31	C	4.048911	10.53053	1.960077
32	H	3.44338	11.25011	1.413283
33	C	5.612676	8.624372	3.423211
34	C	7.807716	7.933247	4.270217
35	C	3.430672	9.326448	2.43591
36	C	6.194546	9.820922	2.888898
37	C	7.752305	5.255229	2.069779
38	H	7.266966	6.032415	2.642374
39	C	4.729778	7.65175	9.870786
40	H	5.526789	7.556259	10.60091
41	C	4.435844	6.283531	4.407409
42	H	3.918326	5.398272	4.766771

43	C	5.37527	10.7599	2.176293
44	H	5.84638	11.666	1.801034
45	C	3.634328	7.18365	3.636622
46	C	7.015057	0.627834	4.480409
47	H	5.961745	0.561453	4.233432
48	C	9.743943	0.725673	5.054457
49	H	10.80655	0.776932	5.276114
50	C	7.214823	1.962944	8.326319
51	H	6.216709	2.181653	7.962739
52	C	8.984142	4.598548	0.089374
53	H	9.467726	4.855926	-0.84969
54	C	9.660499	9.518442	7.594613
55	H	10.74541	9.496138	7.525227
56	C	8.970768	3.273152	0.534452
57	H	9.439807	2.491665	-0.05826
58	C	6.63432	4.831038	10.03553
59	H	5.840384	4.366298	9.459785
60	C	9.81228	1.371993	9.270988
61	H	10.81337	1.144376	9.628084
62	C	8.808155	7.086138	4.880377
63	H	9.843144	7.419068	4.805224
64	C	2.075452	9.039078	2.193784
65	H	1.47413	9.754467	1.637029
66	C	6.876482	9.544962	7.764911
67	H	5.794404	9.575553	7.830319
68	C	2.654485	7.917519	8.024736
69	H	1.854449	8.017609	7.295792
70	C	7.57139	10.04599	3.05182
71	H	8.020756	10.94905	2.644944
72	C	8.976708	10.73737	7.564941
73	H	9.525903	11.67143	7.476296
74	C	8.369025	5.587167	0.859326
75	H	8.365536	6.621875	0.52643
76	C	2.441594	8.265021	9.359777
77	H	1.471823	8.636426	9.681676
78	C	9.587624	2.455727	8.425989
79	C	4.768997	3.317361	2.150622
80	H	5.450843	3.822093	1.475612
81	C	4.249773	2.36234	4.304504
82	H	4.520652	2.114837	5.324804
83	C	3.485027	8.131846	10.28171
84	H	3.332211	8.401129	11.3239
85	C	2.275156	6.929085	3.364203
86	H	1.831183	6.00181	3.719759
87	C	7.582705	10.7452	7.642272
88	H	7.037151	11.68483	7.609032

89	C	7.001268	4.265665	11.25645
90	H	6.502248	3.363529	11.5994
91	C	8.349764	9.110584	3.702943
92	H	9.419749	9.280289	3.794714
93	C	7.439366	0.871529	9.167214
94	H	6.600973	0.240374	9.452086
95	C	9.080155	-0.50539	5.055246
96	H	9.623248	-1.42013	5.278534
97	C	1.506294	7.849089	2.652449
98	H	0.458202	7.639271	2.452583
99	C	7.716464	-0.54976	4.764198
100	H	7.189958	-1.50093	4.750544
101	C	2.58625	2.337502	2.544348
102	H	1.590629	2.080661	2.191495
103	C	3.487512	2.987334	1.699114
104	H	3.197228	3.244335	0.683559
105	C	2.973283	2.024373	3.850715
106	H	2.282215	1.522324	4.523098
107	C	8.015545	4.846216	12.02359
108	H	8.307533	4.401427	12.97148
109	C	8.651011	5.999488	11.56098
110	H	9.439643	6.463689	12.14803
111	C	8.723834	0.575774	9.645421
112	H	8.879667	-0.27645	10.30136

Table S19 Gas phase optimized coordinates of **3b**

Tag	Symbol	X	Y	Z
1	Ru	3.109259	14.84787	13.90033
2	P	3.064149	13.37543	15.94128
3	P	3.364398	16.39759	11.9383
4	S	5.140626	11.4155	11.52649
5	N	5.186683	14.56693	13.84959
6	O	0.102938	15.13067	13.54495
7	N	3.382941	13.06439	12.58506
8	N	5.671771	13.50503	13.11151
9	C	1.689974	13.50484	17.19564
10	C	4.970586	17.31421	11.83622
11	C	2.262331	16.98002	15.90167
12	H	1.27831	16.6045	15.64572
13	C	3.38108	16.42917	15.28171
14	C	2.962101	11.53412	15.67919
15	C	5.947011	16.47771	15.22612

16	C	6.107329	15.30456	14.4014
17	H	7.111333	14.95223	14.20352
18	C	4.673634	16.9764	15.67517
19	C	4.697048	18.09061	16.61227
20	C	2.111064	17.75813	11.74478
21	C	7.138253	18.24016	16.52734
22	C	4.583462	13.61495	16.96828
23	C	7.17765	17.11674	15.62645
24	C	1.249328	15.03302	13.73558
25	C	4.704617	12.82056	12.52372
26	C	3.227845	15.57837	10.277
27	C	1.824718	12.85112	18.43515
28	H	2.748381	12.33696	18.68186
29	C	6.165193	16.60807	11.60224
30	H	6.151407	15.52776	11.48916
31	C	2.652013	12.13917	11.85665
32	C	2.293694	18.03815	16.84634
33	H	1.362856	18.39873	17.27971
34	C	5.903117	18.68272	16.9987
35	H	5.87347	19.5173	17.69755
36	C	3.492132	18.60055	17.18284
37	H	3.55795	19.42861	17.88502
38	C	5.032861	18.70676	11.99699
39	H	4.129094	19.27679	12.18265
40	C	1.686323	18.18184	10.47281
41	H	2.060296	17.69374	9.579568
42	C	4.56865	14.44495	18.10114
43	H	3.650801	14.93619	18.40742
44	C	0.470317	14.12678	16.90298
45	H	0.316773	14.61421	15.95101
46	C	1.255058	12.08694	11.7249
47	H	0.634149	12.82486	12.22215
48	C	8.482617	16.7172	15.18173
49	H	8.603217	15.90007	14.48263
50	C	4.162722	15.74257	9.242962
51	H	5.053652	16.33989	9.396562
52	C	0.781112	12.84645	19.3602
53	H	0.910869	12.33821	20.31247
54	C	-0.42798	13.48358	19.06023
55	H	-1.24314	13.4777	19.77937
56	C	7.382006	17.28519	11.50295
57	H	8.292265	16.72262	11.31066
58	C	7.43278	18.67314	11.66189
59	H	8.382887	19.19695	11.59574
60	C	8.346565	18.88514	16.94279
61	H	8.267054	19.72879	17.62521

62	C	2.072097	14.82393	10.01984
63	H	1.324867	14.69347	10.79482
64	C	3.429067	11.15296	11.19666
65	C	5.731683	14.65578	18.84627
66	H	5.697384	15.30446	19.71776
67	C	1.608529	18.42161	12.87442
68	H	1.9281	18.12169	13.86443
69	C	6.930324	14.04595	18.46909
70	H	7.834702	14.20994	19.04933
71	C	-0.5811	14.11711	17.82711
72	H	-1.5181	14.60662	17.57384
73	C	9.568663	18.45789	16.49536
74	H	10.48271	18.9521	16.81414
75	C	6.256072	19.3796	11.91596
76	H	6.282709	20.45822	12.04816
77	C	5.80388	13.03766	16.57524
78	H	5.860784	12.43696	15.67229
79	C	2.847129	10.14999	10.42527
80	H	3.463511	9.404976	9.928896
81	C	9.627086	17.35722	15.59728
82	H	10.59091	17.01721	15.22611
83	C	6.963088	13.24097	17.32743
84	H	7.894202	12.77876	17.00917
85	C	0.776628	19.23357	10.33934
86	H	0.457988	19.54206	9.34671
87	C	0.279026	19.88433	11.47182
88	H	-0.43047	20.7013	11.36632
89	C	3.953443	15.15151	7.992465
90	H	4.693317	15.28772	7.207569
91	C	1.858563	14.24115	8.770452
92	H	0.961215	13.65245	8.601492
93	C	2.802725	14.39853	7.75187
94	H	2.64174	13.93787	6.780509
95	C	0.669607	11.08068	10.95387
96	H	-0.41327	11.04836	10.85915
97	C	0.701077	19.47637	12.73889
98	H	0.32576	19.9747	13.62922
99	C	1.453191	10.11638	10.30389
100	H	0.981872	9.340398	9.706847
101	C	1.90616	11.06713	14.88184
102	H	1.247226	11.77179	14.38702
103	C	2.513992	8.770729	15.34232
104	H	2.346318	7.705259	15.20696
105	C	3.781966	10.59227	16.32065
106	H	4.592027	10.91253	16.96559
107	C	1.682355	9.700369	14.71246

108	H	0.865394	9.367705	14.07791
109	C	3.561187	9.222146	16.14813
110	H	4.211618	8.509997	16.65023

Table S20 Gas phase optimized coordinates of **4a**

Tag	Symbol	X	Y	Z
1	Ru	-0.82266	7.038011	12.97844
2	S	3.793747	7.25485	12.88518
3	N	1.276909	6.747577	13.4115
4	N	0.299129	8.304871	11.49719
5	N	1.663009	8.25284	11.6015
6	O	-3.73644	7.476118	12.31396
7	C	2.052752	7.455729	12.57965
8	C	-2.43383	8.733567	15.77134
9	C	-1.1901	10.54225	13.92454
10	C	2.009656	6.015277	14.33087
11	C	1.698971	10.07342	9.354608
12	C	-0.24959	9.052198	10.57578
13	C	3.410256	6.155501	14.21246
14	C	-0.0397	11.41918	7.608797
15	C	-0.57974	10.59654	8.648399
16	C	-1.96982	6.291821	9.253191
17	C	-2.61721	7.31263	12.56558
18	C	1.855176	4.343503	11.30957
19	C	-2.32139	3.964085	11.74565
20	C	1.496113	5.180867	15.32869
21	C	-0.94958	5.439538	9.701165
22	C	0.412939	2.61395	12.17018
23	C	-2.01319	10.51673	8.733499
24	C	-4.5758	8.564141	17.57972
25	C	2.210955	10.87388	8.3503
26	C	1.372778	11.55691	7.459912
27	C	-0.35335	12.92957	5.664373
28	C	2.374165	4.514569	16.17849
29	C	0.570544	3.9113	11.66933
30	C	-2.9506	9.887784	16.37749
31	C	2.949658	3.492882	11.43205
32	C	-3.00609	7.49639	16.08466
33	C	4.287711	5.490167	15.05948
34	C	0.447873	9.003373	15.78949
35	C	0.310047	9.903919	9.53675
36	C	-2.79362	3.173356	10.68846
37	C	-0.07999	4.88618	8.75468
38	C	1.072295	13.03948	5.551282
39	C	-2.11232	6.58479	7.900297
40	C	1.512615	1.765731	12.29802

41	C	-1.23163	6.038396	6.967454
42	C	0.318042	8.735486	17.15699
43	C	3.759104	4.663427	16.05103
44	C	1.707537	9.363436	15.28937
45	C	-3.86575	2.304412	10.87674
46	C	-0.38097	11.63026	14.27025
47	C	-0.90091	12.1142	6.70237
48	C	-2.2406	10.75352	13.01932
49	C	2.78191	2.200362	11.92722
50	C	-2.94573	3.860125	12.99332
51	C	-2.60236	13.47692	4.917676
52	C	2.804074	9.468586	16.13979
53	C	-0.21855	5.187745	7.399093
54	C	-4.06812	7.412005	16.98468
55	C	-2.31558	12.0005	6.823712
56	C	1.894209	12.38273	6.411673
57	C	-2.83345	11.17905	7.873322
58	C	-4.47958	2.207172	12.12483
59	C	-3.14653	12.6875	5.924683
60	C	-1.2216	13.59767	4.788077
61	C	-2.46961	12.01224	12.47207
62	C	-4.01382	9.802943	17.27281
63	C	-0.60569	12.89017	13.71343
64	C	1.419833	8.836156	18.00605
65	C	-1.64695	13.08565	12.81144
66	C	2.663584	9.205489	17.50189
67	C	-4.01541	2.985837	13.18219
68	H	-1.28883	6.037894	14.1656
69	H	-2.4765	9.916106	9.503734
70	H	-3.91111	11.08871	7.978125
71	H	-4.22421	12.59585	6.023809
72	H	-3.25679	14.00228	4.229304
73	H	-0.80266	14.21639	3.99988
74	H	1.48438	13.66084	4.761494
75	H	2.972571	12.47286	6.317112
76	H	3.287616	10.97466	8.245793
77	H	2.365485	9.554432	10.02438
78	H	-2.67421	6.717299	9.958283
79	H	-2.90705	7.248225	7.575401
80	H	-1.336	6.275838	5.913759
81	H	0.470045	4.751304	6.682412
82	H	0.707706	4.211034	9.063241
83	H	2.006426	5.345359	10.92505
84	H	3.935291	3.846996	11.14858
85	H	3.636974	1.539675	12.02822
86	H	1.371376	0.762761	12.68833
87	H	-0.56736	2.255131	12.45891
88	H	0.423101	5.066786	15.42342
89	H	1.974622	3.868191	16.95358
90	H	4.427658	4.135414	16.72285
91	H	5.361068	5.610067	14.95371

92	H	-0.64219	8.449317	17.56857
93	H	1.300585	8.623666	19.06379
94	H	3.520649	9.281802	18.16331
95	H	3.770484	9.746742	15.73252
96	H	1.837307	9.570202	14.2333
97	H	-2.52682	10.85866	16.14861
98	H	-4.4046	10.70704	17.72899
99	H	-5.40701	8.499537	18.27476
100	H	-4.50201	6.443759	17.21376
101	H	-2.61926	6.60034	15.61571
102	H	-1.32459	8.997172	10.61916
103	P	-0.85424	5.079018	11.52126
104	P	-0.97692	8.833859	14.62552
105	H	-2.32925	3.237493	9.711378
106	H	-4.22231	1.704527	10.04537
107	H	-5.31737	1.532442	12.26973
108	H	-4.48999	2.920657	14.15625
109	H	-2.59385	4.472263	13.81428
110	H	-2.9013	9.938286	12.74998
111	H	-3.28838	12.15282	11.77401
112	H	-1.81851	14.06466	12.376
113	H	0.038211	13.71859	13.99163
114	H	0.426165	11.50926	14.98102

Table S21 Gas phase optimized coordinates of **5a**

Tag	Symbol	X	Y	Z
1	C	6.769653	11.70859	14.74885
2	C	5.435121	11.78627	15.17675
3	C	4.931429	12.96902	15.713
4	C	5.754792	14.08452	15.85541
5	C	7.086248	14.00977	15.456
6	C	7.590115	12.83291	14.90407
7	Ru	7.537779	8.229357	15.65243
8	P	7.591561	6.426026	17.36125
9	P	7.432842	10.12806	14.04742
10	S	3.14401	7.093513	14.58721
11	N	5.851068	9.013598	16.60379
12	N	4.590912	8.63256	16.24181
13	O	9.963413	7.07008	14.22681
14	C	7.423093	10.20768	17.85584
15	N	5.762112	7.274959	14.65858
16	C	9.228513	5.635616	17.74415
17	C	6.049115	9.878021	17.55354
18	C	4.652746	7.750833	15.25059
19	C	5.656455	7.2902	19.23802
20	C	6.409174	9.830629	12.52804

21	C	9.056292	7.522684	14.78296
22	C	6.59176	4.912733	16.96429
23	C	9.018479	10.6803	13.25604
24	C	8.418178	9.533733	17.06899
25	C	7.767383	11.13983	18.8686
26	C	6.999682	6.934899	19.04052
27	C	10.13997	10.74809	18.34955
28	C	9.283704	4.345364	18.29321
29	C	10.42525	6.327876	17.54281
30	C	11.69402	4.467544	18.4167
31	C	11.64983	5.749272	17.87617
32	C	9.145719	11.41225	19.11976
33	C	6.924442	4.215113	15.79599
34	C	7.166368	12.72307	20.63492
35	C	11.40851	11.59713	12.09909
36	C	9.744924	9.835227	17.35216
37	C	11.51946	11.03059	18.61462
38	C	5.58544	4.396936	17.78815
39	C	7.882597	7.020557	20.12373
40	C	9.002569	11.37823	12.03877
41	C	5.207084	7.688438	20.4948
42	C	6.798359	11.83731	19.67011
43	C	10.5058	3.767572	18.62526
44	C	5.469833	6.370428	13.65549
45	C	10.18768	11.83075	11.46589
46	C	4.922421	3.218274	17.44419
47	C	11.89364	11.91445	19.5804
48	C	8.544386	13.01055	20.90676
49	C	11.43419	10.91037	13.30939
50	C	10.91725	12.60174	20.37431
51	C	11.27249	13.5187	21.37656
52	C	4.091016	6.129837	13.45328
53	C	6.093192	7.763092	21.56814
54	C	3.633945	5.246888	12.4831
55	C	10.24662	10.45543	13.88218
56	C	8.946846	13.91876	21.89691
57	C	9.534753	12.3395	20.13117
58	C	6.392035	5.693635	12.84835
59	C	7.432468	7.434668	21.37649
60	C	6.269071	3.03599	15.45769
61	C	5.261386	2.534411	16.28032
62	C	6.811713	8.786481	11.68509
63	C	5.044908	9.311869	10.12743
64	C	10.29755	14.16815	22.12734
65	C	4.568903	4.581623	11.68859
66	C	5.315753	10.61514	12.14654
67	C	6.139779	8.530804	10.49476
68	C	5.93637	4.808099	11.87599
69	C	4.636228	10.35258	10.95616
70	H	5.318691	4.897661	18.70914
71	H	4.142101	2.836174	18.09486

72	H	4.74437	1.618191	16.0137
73	H	6.537745	2.517546	14.54357
74	H	7.707561	4.587693	15.14622
75	H	10.40418	7.327594	17.13598
76	H	12.56784	6.303406	17.7088
77	H	12.64644	4.014646	18.67319
78	H	10.52858	2.767188	19.04579
79	H	8.372094	3.784385	18.46083
80	H	4.952633	7.262252	18.41399
81	H	4.162078	7.94985	20.62912
82	H	5.743127	8.082112	22.54467
83	H	8.134481	7.500087	22.20147
84	H	8.927543	6.766392	19.99754
85	H	5.74255	11.65953	19.50668
86	H	6.40622	13.23215	21.22103
87	H	8.19121	14.4297	22.48679
88	H	10.59165	14.87392	22.89787
89	H	12.32394	13.71856	21.56223
90	H	12.94578	12.11304	19.7644
91	H	12.27393	10.51911	18.02274
92	H	10.54587	9.359166	16.79233
93	H	2.57123	5.076619	12.34463
94	H	4.230596	3.888646	10.92551
95	H	6.656652	4.286058	11.2535
96	H	7.453691	5.863791	12.98576
97	H	4.780092	10.92572	15.10155
98	H	3.89378	13.01138	16.02908
99	H	5.362718	15.00251	16.28147
100	H	7.740756	14.86747	15.57294
101	H	8.628127	12.79959	14.59739
102	H	7.665206	8.173113	11.95055
103	H	6.4653	7.71276	9.861142
104	H	4.515315	9.108994	9.20213
105	H	3.787957	10.97058	10.67915
106	H	4.992033	11.44388	12.76196
107	H	10.27699	9.931935	14.82565
108	H	12.37805	10.72245	13.81101
109	H	12.33213	11.94783	11.6497
110	H	10.15643	12.36606	10.5222
111	H	8.064152	11.56769	11.53135
112	H	5.188421	10.29852	18.0615