Electronic Supplementary Information

For

Steric control on the coordination behaviour of carbazole thiosemicarbazones towards $[RuH(Cl)(CO)(AsPh_3)_3]$: A combined experimental and theoretical studies

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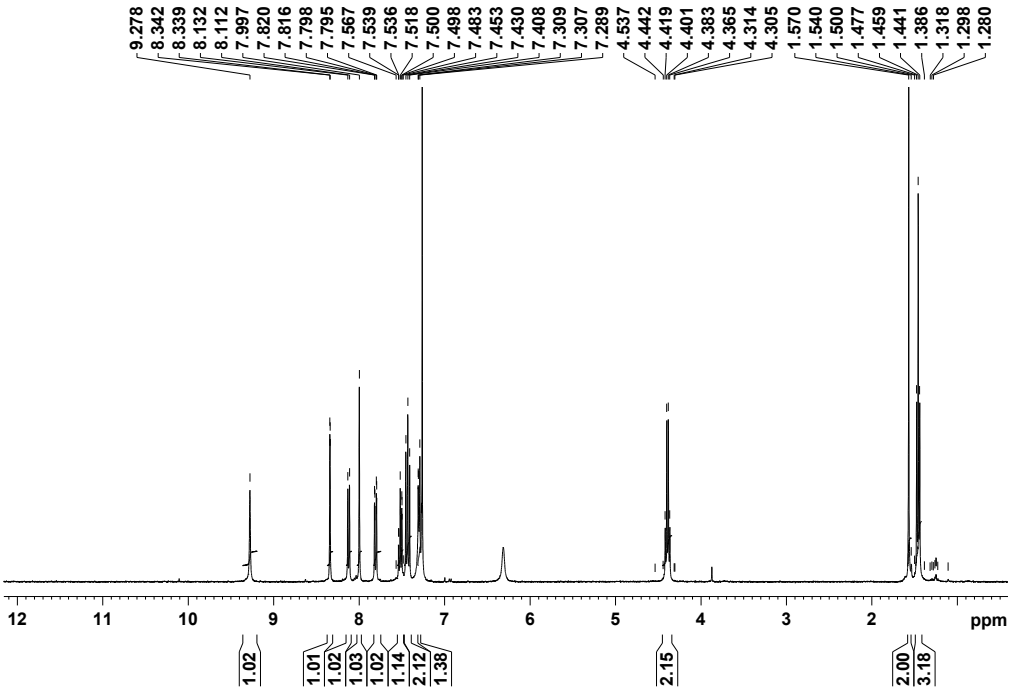

Fig.S1(i) ^{1}H NMR spectrum of the ligand-L1 in $CDCl_3$ solution

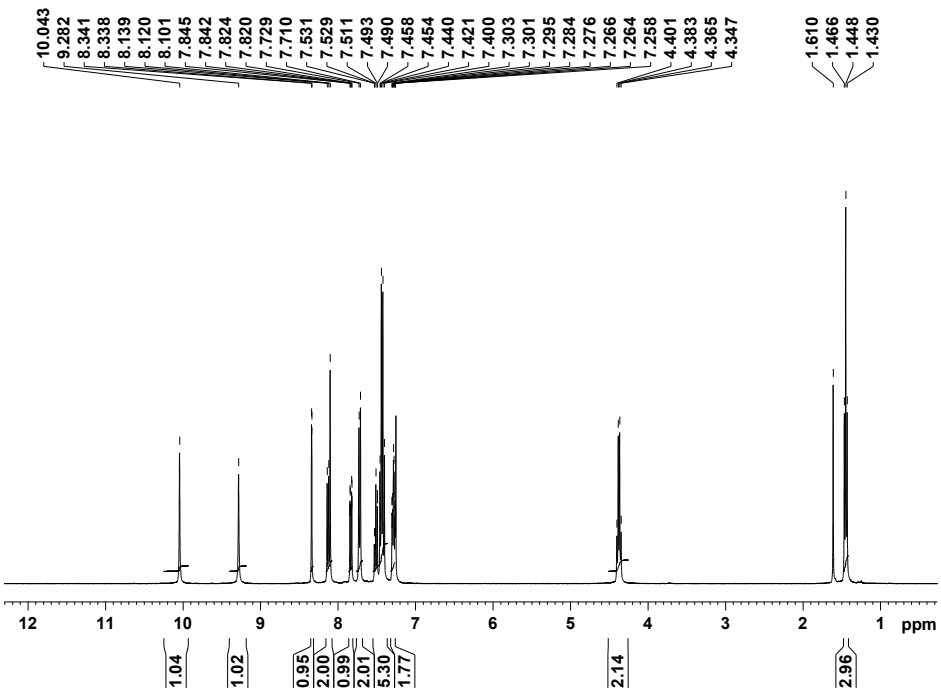

Fig.S1(ii) ^{1}H NMR spectrum of the ligand-L2 in $CDCl_3$ solution

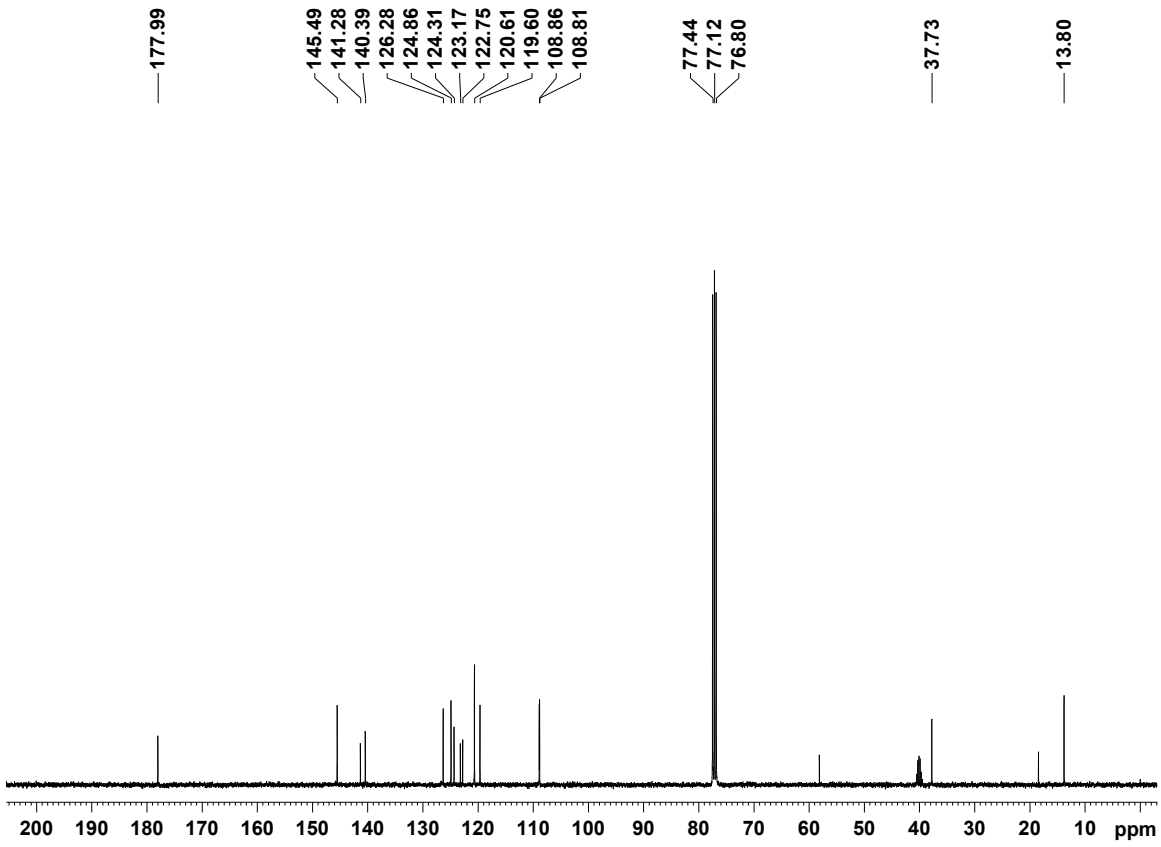

Fig.S2(i) ^{13}C NMR spectrum of the ligand-L1 in $CDCl_3$ solution

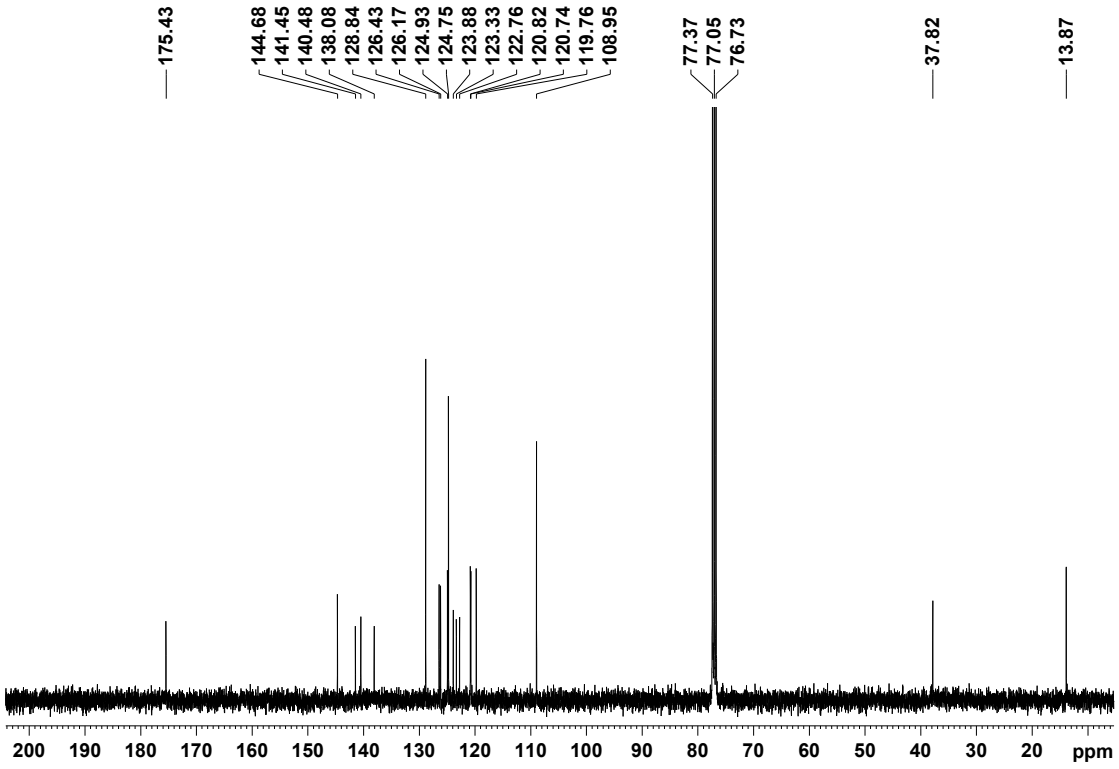

Fig.S2(ii) ^{13}C NMR spectrum of the ligand-L2 in $CDCl_3$ solution

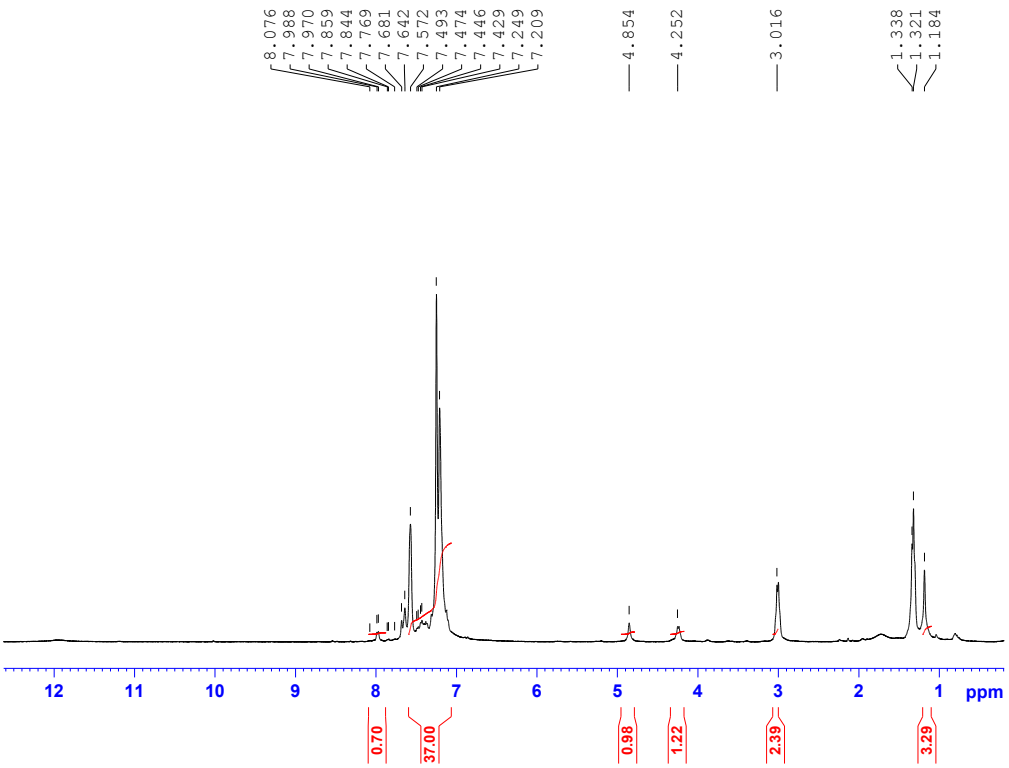

Fig.S3(i) ^{1}H NMR spectrum of the complex-1 in $CDCl_3$ solution

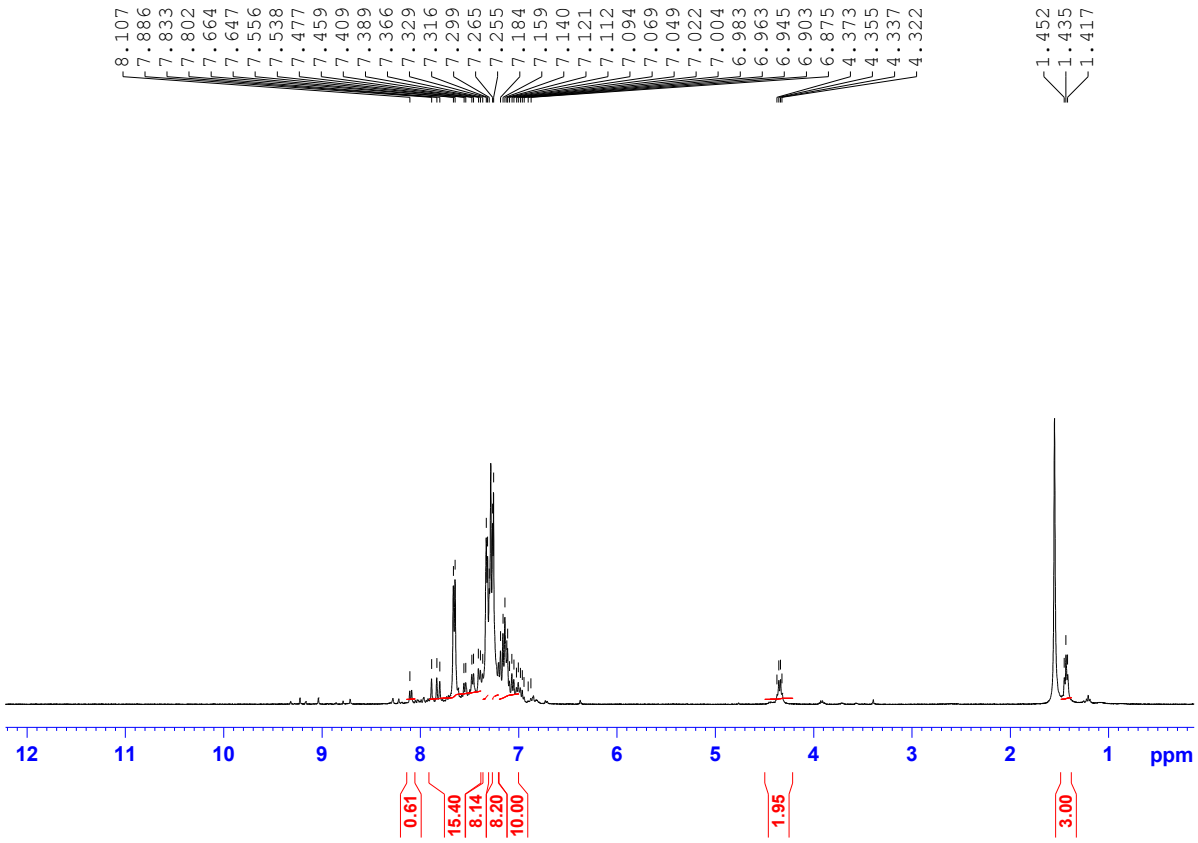

Fig.S3(ii) ^{1}H NMR spectrum of the complex-2 in $CDCl_3$ solution

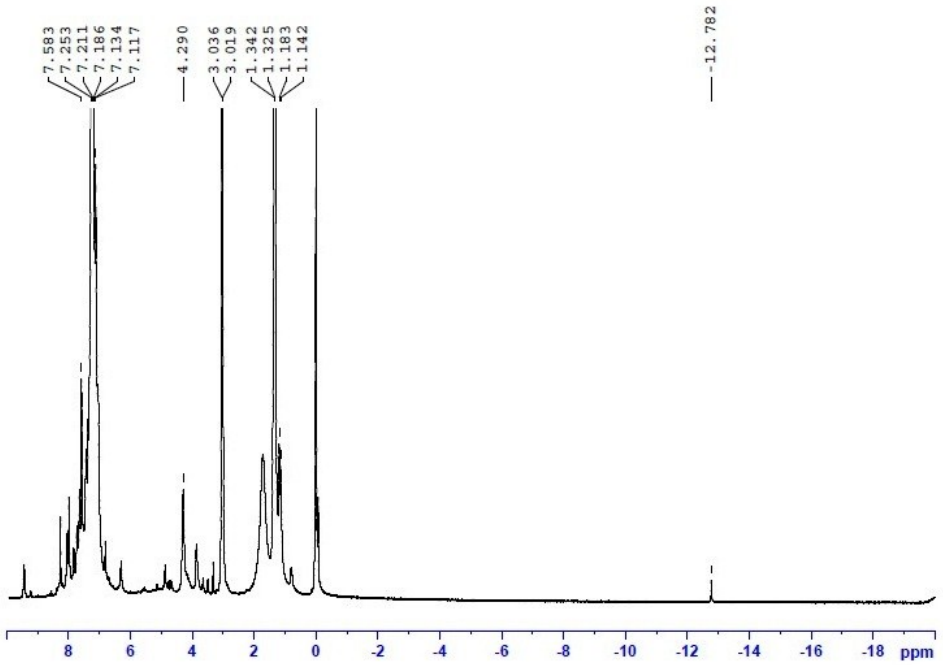

Fig.S4(i) ^{1}H NMR spectrum of the complex-1 in $CDCl_3$ solution at negative region

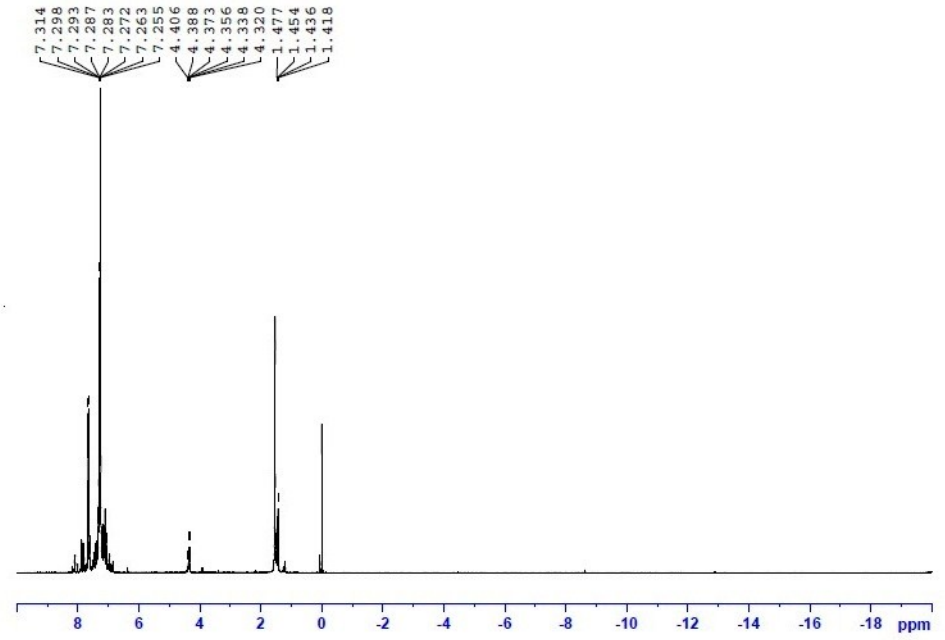

Fig.S4(ii) ^{1}H NMR spectrum of the complex-2 in $CDCl_3$ solution at negative region

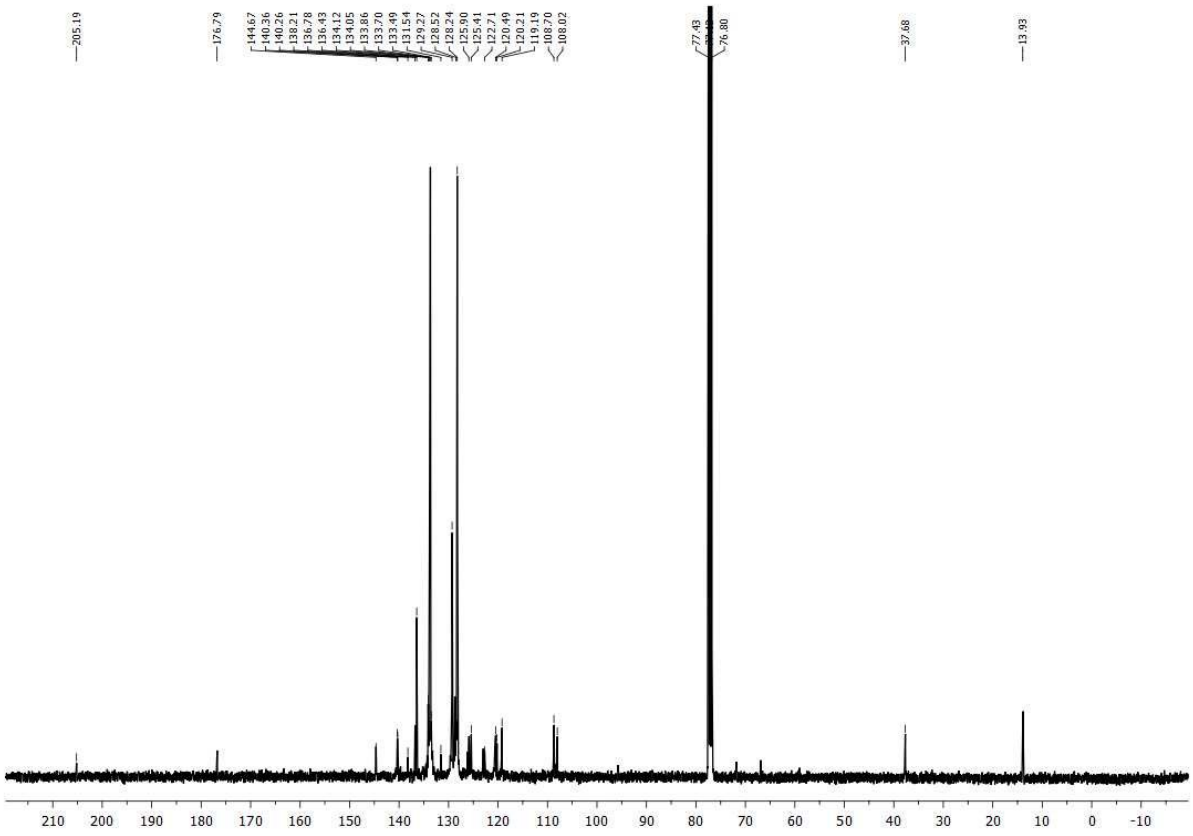

Fig.S5(i) ^{13}C NMR spectrum of the complex-1 in $CDCl_3$ solution

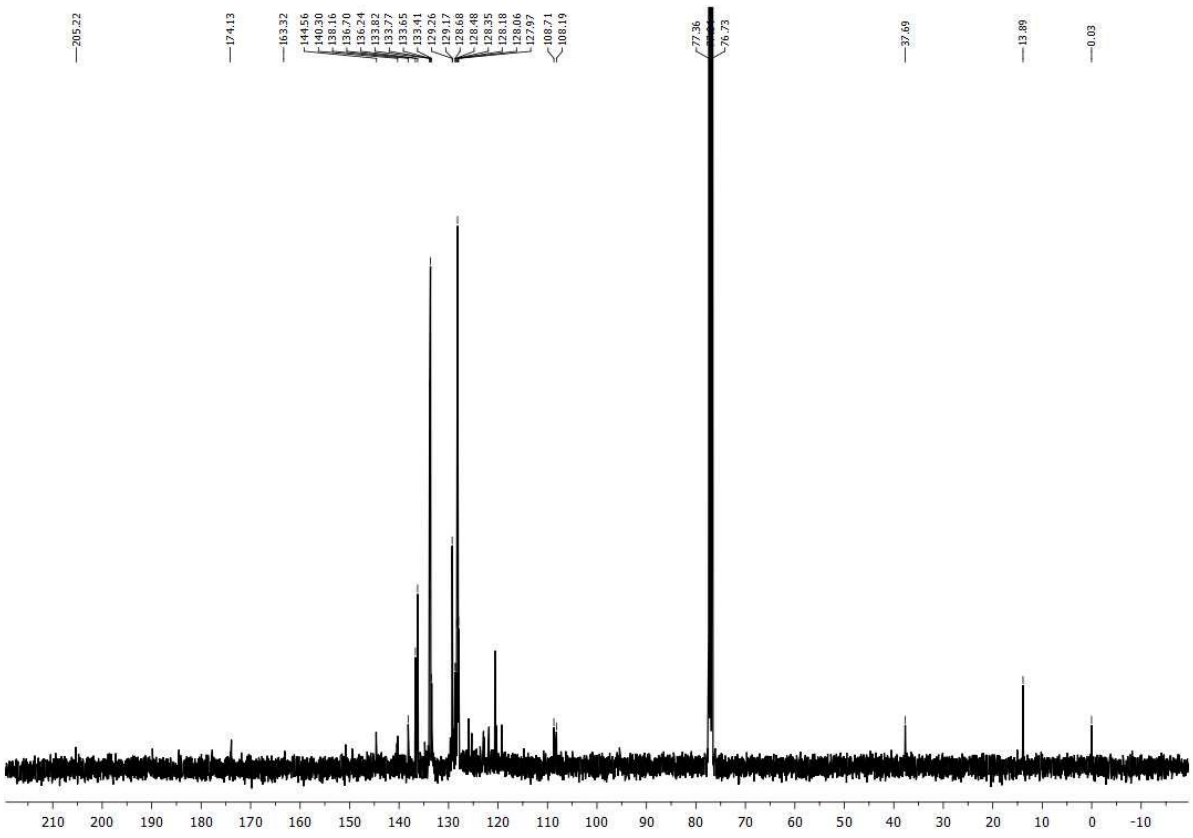

Fig.S5(ii) ^{13}C NMR spectrum of the complex-2 in $CDCl_3$ solution

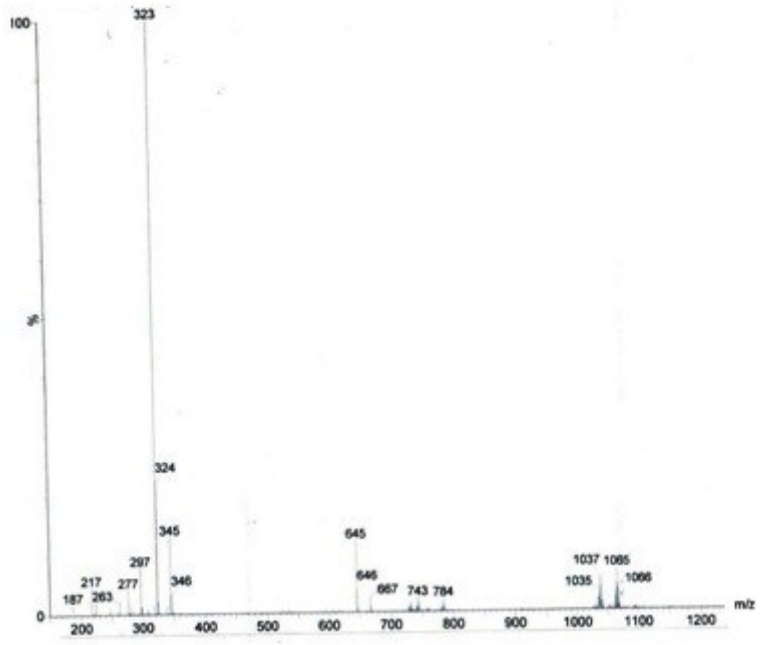

Fig.S6(i) Mass spectrum of the complex-1

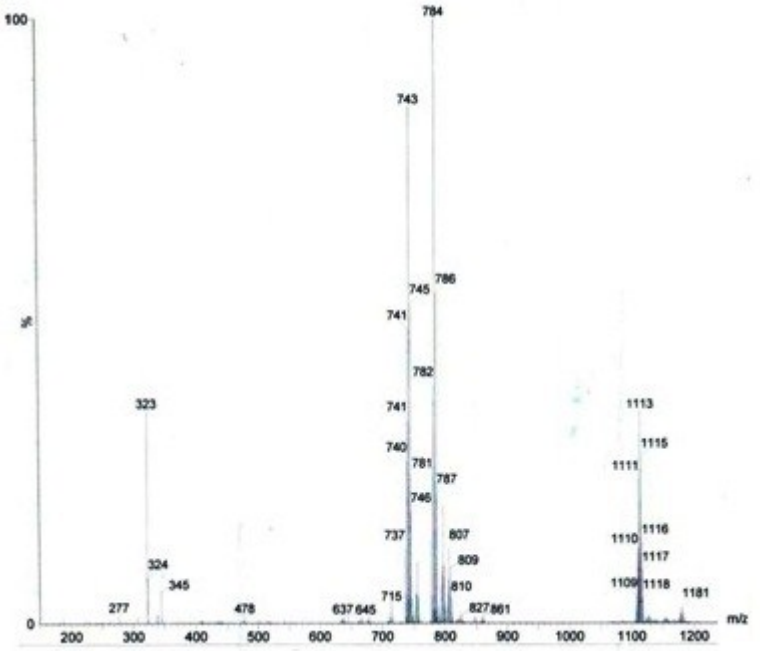

Fig. S6(ii) Mass spectrum of the complex-2

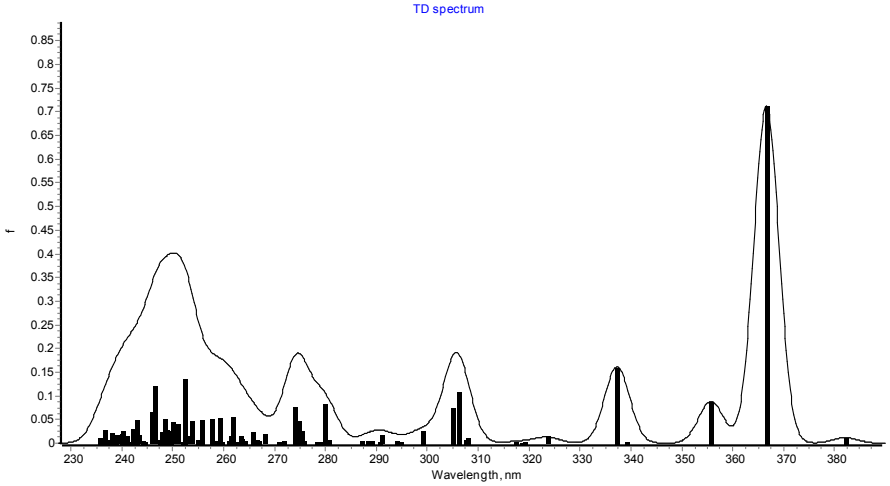

Fig. S7 TD- DFT spectrum of the complex-1

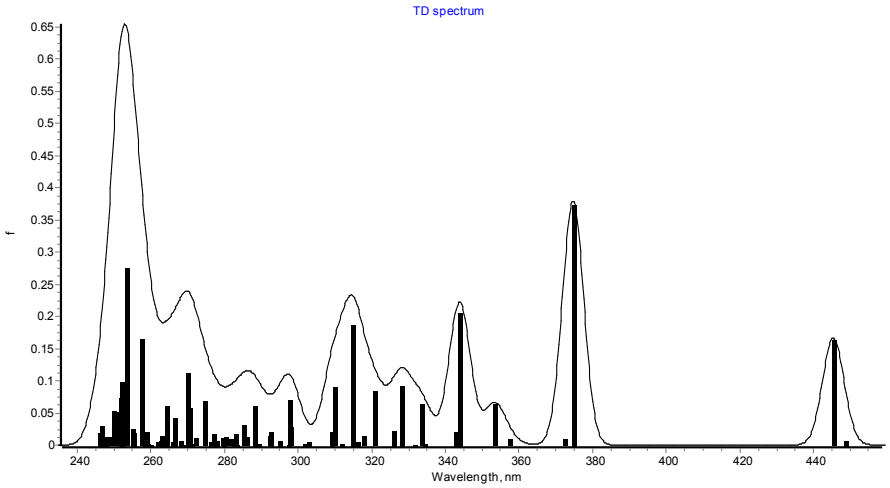

Fig. S8 TD- DFT spectrum of the complex-2.

Table S1. Crystal data and structure refinement parameters for complexs 1 and 2

	Complex **1**	Complex **2**.CH_3CN
Empirical formula	$C_{53}H_{46}As_2N_4ORuS$	$C_{59}H_{48}As_2N_4ORuS$
Formula weight	1037.91	1153.04
Colour	Red	Yellow
Temperature (K)	296(2)	295(2)
Wavelength (Å)	0.71073	0.71073
Crystal system	Monoclinic	Triclinic
Space group	P_{21}/n	P_1
a (Å)	15.7722(7)	12.3121(7)
b (Å)	17.7021(7)	13.7064(7)
c (Å)	17.7700(7)	17.7353(9)
α (°)	90	86.508(4)
β (°)	97.681(2)	71.243(5)
γ (°)	90	67.212(5)
Volume ($Å^3$)	4916.9(4)	2605.8(3)
Z	4	2
$\rho_{calcd.}$ (Mg m^{-3})	1.402	1.470
μ (mm^{-1})	1.738	1.648
F(000)	2104	1172
Crystal size (mm)	0.10x 0.12 x 0.14	0.03x0.26x 0.30
Theta range (°)	1.738 to 28.009	4.0480 to 29.4310
Limiting indices	$-20 \le h \le 17$,	$-15 \le h \le 17$,
	$-21 \le k \le 23$,	$-19 \le k \le 16$,
	$-23 \le l \le 19$	$-20 \le l \le 24$
Reflections collected/unique	11163/6775	12414/8113
Data/restraints/parameters	11163/0/565	12414/0/642
Final *R* indices [$I>2\sigma(I)$]	R_1 =0.0969,	R_1 =0.0686,
	wR_2 = 0.0698	wR_2 = 0.0412
R indices (all data)	R_1 =0.1288,	R_1 =0.998,
	wR_2 = 0.1126	wR_2 = 0.846
Largest diff. peak and hole	1.024, -0.803	1.024 ,-0.803

Table S2. Selected bond lengths (Å) and bond angles (°) for complexs 1 and 2

Complex **1**		Complex **2**	
Bond Length (Å)		Bond Length (Å)	
Ru1-H	1.62(4)	Ru1—As1	2.4372(5)
Ru1-As1	2.4259(5)	Ru1—As2	2.4481(5)
Ru1-As2	2.4284(6)	Ru1—S1	2.5378(11)
Ru1-S1	2.5378(11)	Ru1—N1	2.087(3)
Ru1-N1	2.146(4)	Ru1—C1	1.846(4)
Ru1-C1	1.828(6)	Ru1—C5	2.069(4)
Bond Angle (°)		Bond Angle (°)	
As1-Ru1-H	86.6(15)	As1—Ru1—As2	176.777(17)
As1-Ru1-As2	174.37(2)	As1—Ru1—S1	90.43(3)
As1-Ru1-S1	90.74(3)	As2—Ru1—S1	91.45(3)
As2-Ru1-S1	94.31(3)	N1—Ru1—As1	86.66(10)
N1-Ru1-As1	89.19(9)	N1—Ru1—As2	94.30(10)
N1-Ru1-As2	90.73(9)	N1—Ru1—S1	77.57(9)
N1-Ru1-S1	64.58(9)	C1—Ru1—As1	89.14(13)
S1-Ru1-H	158.5(18)	C1—Ru1—As2	87.84(13)
N1-Ru1-H	94.0(17)	C1—Ru1—S1	105.53(14)
C1-Ru1-H	91.3(17)	C5—Ru1—N1	79.47(14)

Table S3. Selected bond lengths [Å] and angles [º] for L1, L2, C1 and C2 with the optimized geometry values.

	L1		L2	
Bond lengths(Å)	**Exp.**	**Calc.**	**Exp.**	**Calc.**
S(1)-C(1)	1.688(4)	1.70	1.687(3)	1.77
N(1)-N(2)	1.375(4)	1.48	1.379(3)	1.37
N(1)-C(1)	1.340(5)	1.42	1.347(3)	1.31
N(2)-C(2)	1.277(5)	1.35	1.276(3)	1.30
N(3)-C(1)	1.318(5)	1.43	1.343(3)	1.38
N(3)-C(17)			1.415(4)	1.41
N(4)-C(11)	1.375(6)	1.42	1.383(4)	1.39
N(4)-C(12)	1.384(5)	1.43	1.383(4)	1.39
N(4)-C(15)	1.452(6)	1.50	1.507(5)	1.46
C(1)-N(1)-N(2)	119.9(3)	118.3	119.3(2)	114.2
C(2)-N(1)-N(2)	115.6(3)	108.3	116.5(2)	117.9
C(1)-N(3)-C(17)			126.9(2)	132.2
C(11)-N(4) C(12)	108.4(3)	106.8	108.2(2)	108.8
C(11)-N(4) C(15)	126.0(4)	125.8	126.5(3)	126.1
C(12)-N(4) C(15)	125.6(4)	125.7	124.4(3)	125.0
N(1)-C(1)-S(1)	120.1(3)	117.7	119.8(2)	113.6
N(3)-C(1)-S(1)	123.4(3)	123.9	125.2(2)	126.6
N(3)-C(1)-N(1)	116.5(4)	118.3	115.0(2)	114.2
N(2)-C(2)-C(3)	122.5(4)	121.4	121.7(3)	117.7
Bond angles (°)	**complex 1**		**compound 2**	
Ru(1)-H(1)	1.62(4)	1.61		
Ru(1)-As(1)	2.4259(5)	2.51	2.4372(5)	2.53
Ru(1)-As(2)	2.4284(6)	2.51	2.4481(5)	2.54
Ru(1)-S(1)	2.5378(11)	2.66	2.4680(12)	2.55
Ru(1)-N(1)	2.146(4)	2.19	2.087(3)	2.13
Ru(1)-C(1)	1.828(6)	1.86	1.846(4)	1.87
Ru(1)-C(5)			2.069(4)	2.10
C(1)-O(1)	1.147(6)	1.17	1.145(5)	1.17
C(2)-S(1)			1.740(5)	1.77
As(1)-Ru(1)-H(1)	86.6(15)	88.1		
As(1)-Ru(1)-As(2)	174.37(2)	176.1	176.777(17)	177.5
As(1)-Ru(1)-S(1)	90.74(3)	91.2	90.43(3)	88.9
As(2)-Ru(1)-H(1)	87.7(15)	88.2		
As(2)-Ru(1)-S(1)	94.31(3)	92.7	91.45(3)	89.2
S(1)-Ru(1)-H(1)	158.5(18)	160.2		
N(1)-Ru(1)-H(1)	94.0(17)	97.0		
N(1)-Ru(1)-As(1)	89.19(9)	90.5	88.66(10)	90.0
N(1)-Ru(1)-As(2)	90.73(9)	90.7	94.30(10)	91.0
N(1)-Ru(1)-S(1)	64.58(9)	63.2	77.57(9)	77.0
C(1)-Ru(1)-H(1)	91.3(17)	86.9		
C(1)-Ru(1)-As(1)	90.68(15)	89.0	89.14(13)	89.7
C(1)-Ru(1)-As(2)	89.91(15)	90.0	87.84(13)	89.5
C(1)-Ru(1)-S(1)	110.15(14)	112.8	105.53(14)	108.4
C(1)-Ru(1)-N(1)	174.73(16)	176.1	176.21(15)	174.6
C(5)-Ru(1)-As(1)			97.46(17)	91.7
C(5)-Ru(1)-As(2)			90.17(11)	90.7
C(5)-Ru(1)-S(1)			157.01(11)	156.1
C(5)-Ru(1)-N(1)			79.47(14)	79.0

Table S4. Composition of the selected molecular orbitals of complex 1 and 2.

	complex 1					complex 2			
	Ru	CO	L1	$AsPh_3$	H(Ru)	Ru	L2	CO	$AsPh_3$
L+10	0	0	0	100	0	0	2	0	98
L+9	0	0	0	100	0	0	1	0	99
L+8	0	0	0	100	0	0	0	0	99
L+7	1	0	0	99	0	0	0	0	100
L+6	2	0	0	98	0	1	3	0	96
L+5	1	0	0	99	0	3	0	0	97
L+4	1	0	0	99	0	1	1	0	98
L+3	2	0	0	98	0	0	1	0	99
L+2	2	0	1	97	0	1	0	0	98
L+1	0	0	100	0	0	2	0	0	98
LUMO	0	0	99	0	0	3	91	2	4
HOMO	89	0	3	8	0	70	26	1	4
H-1	75	24	1	1	0	72	3	24	1
H-2	70	18	4	7	0	65	15	14	5
H-3	3	0	96	1	0	18	77	2	3
H-4	1	0	97	2	0	1	96	0	2
H-5	19	1	74	2	4	4	95	0	1
H-6	9	2	85	1	2	11	87	0	1
H-7	1	0	97	1	0	2	97	0	1
H-8	1	0	91	7	0	15	82	1	2
H-9	5	1	9	84	0	0	99	0	1
H-10	13	1	2	72	12	0	99	0	1

Table S5. The calculated electronic transition for [RuH(CO)(Ash_3)$_2$(L1)] complex

Wavelength (nm)	Osc. Strength	Major contributions
382.0161351	0.0117	H-1->L+1 (35%), HOMO->L+1 (35%)
366.6085237	0.7121	HOMO->LUMO (92%)
355.7423868	0.088	H-1->L+1 (18%), HOMO->L+1 (52%)
339.2064147	0.002	HOMO->L+3 (53%), HOMO->L+5 (15%)
337.259498	0.1601	HOMO->L+2 (84%)
323.5388864	0.0127	H-1->LUMO (93%)
319.0923604	0.0018	H-1->L+3 (12%), HOMO->L+3 (19%), HOMO->L+4 (25%)
318.6495069	0.0008	HOMO->L+3 (12%), HOMO->L+4 (67%)
317.198395	0.0019	H-1->L+3 (11%), HOMO->L+5 (62%)
307.849572	0.0108	HOMO->L+6 (73%)
307.3078117	0.008	H-4->L+1 (56%)
306.0636813	0.1085	H-2->LUMO (56%)
304.8220894	0.0747	H-2->LUMO (19%), HOMO->L+7 (11%)
299.0865457	0.0265	HOMO->L+6 (11%), HOMO->L+7 (24%)
294.7212528	0.0028	HOMO->L+7 (48%), HOMO->L+8 (21%), HOMO->L+9 (18%)
293.9456522	0.0054	HOMO->L+8 (33%), HOMO->L+9 (55%)
290.8768221	0.016	H-4->L+3 (20%), H-1->L+4 (22%)
290.7472191	0.0016	HOMO->L+10 (78%)
288.9987101	0.0038	H-4->LUMO (56%), H-3->LUMO (22%)
288.8505851	0.0001	H-4->LUMO (11%), H-3->LUMO (12%), H-1->L+2 (27%), H-1->L+4 (17%)
288.2461968	0.0046	H-4->LUMO (10%), H-1->L+4 (38%)
286.9785354	0.0036	H-1->L+3 (17%), H-1->L+5 (39%)
280.5306739	0.0074	H-1->L+3 (17%), H-1->L+6 (27%)
279.7647328	0.0819	H-3->LUMO (37%), H-1->L+2 (41%)
279.0720432	0.0015	HOMO->L+11 (80%)
278.2390858	0.0023	H-5->L+1 (12%), H-2->L+1 (24%), H-1->L+5 (11%)
275.5920171	0.0041	H-1->L+6 (23%), HOMO->L+12 (17%)
275.1394449	0.0264	H-2->L+2 (13%), HOMO->L+13 (50%)
274.51806	0.0464	H-2->L+2 (11%), H-1->L+6 (11%), HOMO->L+12 (41%)

274.4694427	0.0272	H-2->L+2 (10%), H-1->L+6 (13%), HOMO->L+13 (11%), HOMO->L+14 (22%)
273.9842143	0.0765	H-5->LUMO (10%), H-2->L+2 (17%), HOMO->L+13 (17%), HOMO->L+14 (17%)
271.7919562	0.0045	HOMO->L+12 (17%), HOMO->L+14 (34%)
270.6764254	0.0023	H-14->LUMO (20%), H-10->LUMO (10%), H-9->LUMO (10%), H-8->LUMO (18%)
267.8809425	0.0192	H-1->L+7 (25%)
266.9580704	0.004	H-5->LUMO (10%), H-3->L+1 (17%), H-1->L+7 (25%)
266.3616058	0.008	H-1->L+7 (11%), H-1->L+8 (17%), HOMO->L+15 (39%)
265.608382	0.0241	H-5->LUMO (35%)
264.1371496	0.0038	H-4->L+4 (27%), H-1->L+8 (11%)
263.5083986	0.0087	H-4->L+4 (14%), H-1->L+9 (33%)
263.295752	0.0127	H-1->L+9 (11%), HOMO->L+16 (23%)
262.7322243	0.0033	H-2->L+3 (37%)
261.8388981	0.056	H-3->L+2 (35%), H-2->L+4 (11%), HOMO->L+17 (11%)
261.4137991	0.0134	H-2->L+4 (60%)
260.8802454	0.0042	H-1->L+10 (75%)
259.5639925	0.0034	H-2->L+5 (50%)
259.1570758	0.0533	H-7->LUMO (18%), H-6->LUMO (11%), HOMO->L+17 (15%)
258.4547678	0.0043	H-4->L+3 (14%), H-4->L+5 (24%), H-2->L+5 (18%)
257.7133938	0.0518	H-7->LUMO (26%), H-6->L+1 (13%)
255.772861	0.0483	H-7->L+1 (22%), H-6->LUMO (21%), H-1->L+11 (13%)
254.8318431	0.0072	H-7->LUMO (19%), H-6->LUMO (41%), H-1->L+11 (19%)
253.4928167	0.047	H-3->L+3 (12%), H-2->L+6 (22%), H-1->L+11 (22%)
252.655968	0.0139	H-4->L+4 (10%), H-4->L+6 (15%), H-2->L+6 (12%)
252.4039344	0.0364	H-3->L+3 (12%), H-2->L+6 (35%)
252.301208	0.1356	H-6->L+1 (15%), H-3->L+3 (10%)
251.7939412	0.003	H-4->L+2 (80%)
250.9073069	0.0393	H-3->L+3 (28%), H-1->L+14 (10%)
249.9815244	0.0443	H-5->L+4 (12%), H-4->L+4 (10%), H-3->L+4 (41%)
249.604076	0.0248	H-5->L+3 (21%), H-3->L+4 (11%)
249.247807	0.0105	H-1->L+12 (32%), H-1->L+13 (35%)

248.8026502	0.0281	H-1->L+12 (16%), H-1->L+14 (23%), H-1->L+15 (16%)
248.4287508	0.0501	H-4->L+5 (13%), H-4->L+6 (35%)
247.8823933	0.0223	H-1->L+12 (13%), H-1->L+13 (32%), H-1->L+15 (15%)
247.3285656	0.0074	H-3->L+5 (45%)
246.5171524	0.1209	H-2->L+7 (22%), HOMO->L+17 (14%)
245.9254917	0.0657	H-2->L+7 (34%), H-2->L+9 (12%)
244.4514613	0.0012	H-2->L+8 (19%), H-2->L+9 (45%)
244.229955	0.0036	H-5->L+4 (11%), HOMO->L+17 (10%)
243.3383773	0.0164	H-4->L+7 (24%), H-2->L+10 (11%)
242.7666124	0.0485	H-6->L+3 (18%)
242.2732519	0.0057	H-8->LUMO (19%), H-2->L+8 (11%), H-2->L+10 (15%)
242.1502249	0.0191	H-3->L+6 (34%)
242.0178739	0.0302	H-9->LUMO (32%), H-2->L+10 (12%)
241.7394647	0.0011	H-9->LUMO (14%), H-8->LUMO (15%), H-2->L+10 (18%)
241.2549603	0.0019	H-13->LUMO (10%), H-10->LUMO (13%), H-8->L+1 (11%)
240.8753043	0.0149	H-5->L+4 (11%), H-4->L+7 (12%), HOMO->L+18 (10%)
240.3942543	0.0055	H-5->L+4 (23%)
240.1474716	0.0254	H-5->L+2 (68%)
239.9336932	0.0188	H-6->L+3 (11%), H-5->L+2 (13%), H-5->L+5 (13%)
239.8223077	0.001	H-12->LUMO (28%), H-10->LUMO (17%), H-8->L+1 (11%)
238.9809881	0.0172	H-5->L+5 (23%)
238.8290729	0.003	H-4->L+8 (22%), H-4->L+9 (37%)
238.3515709	0.0059	H-13->LUMO (13%), H-9->L+1 (18%)
237.8257819	0.0218	
237.7938523	0.0035	H-6->L+4 (27%)
237.1479823	0.0014	HOMO->L+18 (14%)
237.0074488	0.0079	H-3->L+7 (13%), HOMO->L+18 (17%)
236.6591014	0.0269	
236.4018927	0.0004	H-3->L+7 (10%)
235.7770023	0.0034	H-4->L+10 (41%)
235.5977893	0.0113	H-11->LUMO (25%), H-4->L+10 (14%)

Table S6. The calculated electronic transition for [Ru(CO)(Ash_3)$_2$(L2)] complex

Wavelength (nm)	Osc. Strength	Major contributions
448.5486655	0.0062	H-1->L+1 (12%), HOMO->L+1 (66%)
445.3104541	0.1633	HOMO->LUMO (90%)
374.7418366	0.3726	H-1->LUMO (84%)
372.3335134	0.009	H-1->L+1 (25%), HOMO->L+1 (29%), HOMO->L+3 (13%), HOMO->L+8 (13%)
357.4345912	0.0088	H-1->L+1 (43%), HOMO->L+3 (27%), HOMO->L+8 (12%)
353.2993379	0.0623	HOMO->L+2 (77%)
343.9968277	0.2044	H-2->LUMO (44%), HOMO->L+4 (41%)
342.5521817	0.0197	HOMO->L+3 (30%), HOMO->L+5 (28%), HOMO->L+8 (21%)
334.484411	0.0024	HOMO->L+5 (60%), HOMO->L+8 (14%)
333.6024126	0.063	H-2->LUMO (25%), HOMO->L+4 (24%), HOMO->L+6 (37%)
331.7634975	0.0004	H-3->LUMO (91%)
328.2066302	0.0911	H-3->L+1 (11%), H-2->LUMO (15%), HOMO->L+4 (18%), HOMO->L+6 (42%)
325.7918243	0.0226	H-3->L+1 (60%), HOMO->L+6 (14%)
320.6272121	0.0829	H-2->L+1 (78%)
317.8244979	0.013	H-1->L+2 (18%), H-1->L+4 (10%), HOMO->L+7 (55%)
315.945509	0.0044	H-1->L+3 (52%)
314.8223469	0.1863	H-4->LUMO (10%), H-1->L+2 (41%), HOMO->L+7 (30%)
311.8293175	0.0011	HOMO->L+9 (71%), HOMO->L+11 (15%)
309.7647386	0.0901	H-1->L+4 (20%), HOMO->L+10 (43%)
309.1391229	0.0207	H-1->L+4 (16%), HOMO->L+9 (10%), HOMO->L+10 (18%), HOMO->L+11 (26%)
309.0235454	0.0134	HOMO->L+9 (10%), HOMO->L+10 (34%), HOMO->L+11 (27%)
303.0266079	0.0044	HOMO->L+12 (58%)
301.6846403	0.0022	H-1->L+3 (10%), H-1->L+5 (66%)
298.0010495	0.0266	H-5->L+1 (12%), H-4->L+1 (29%), H-2->L+1 (11%)
297.6719326	0.0689	H-4->LUMO (28%), H-1->L+4 (23%), H-1->L+6 (13%), HOMO->L+12 (15%)
297.3792014	0.0007	H-1->L+3 (13%), H-1->L+5 (20%), H-1->L+8 (35%)
294.9806967	0.0074	H-1->L+6 (61%), HOMO->L+13 (25%)

292.6827427	0.0202	HOMO->L+13 (34%), HOMO->L+14 (29%)
292.3239022	0.0143	HOMO->L+13 (19%), HOMO->L+14 (55%)
289.3629347	0.0025	H-2->L+3 (17%), HOMO->L+11 (11%), HOMO->L+17 (43%)
288.8640447	0.0012	H-2->L+2 (13%), H-1->L+7 (59%)
288.0185301	0.0615	H-3->L+3 (19%), H-3->L+8 (20%), H-1->L+7 (10%)
285.9592145	0.0124	H-2->L+2 (21%), H-2->L+3 (43%), HOMO->L+17 (12%)
285.0847014	0.0312	H-2->L+2 (50%), H-2->L+3 (21%), H-1->L+7 (11%)
283.3127751	0.0008	HOMO->L+15 (86%)
283.0088261	0.0167	H-5->LUMO (65%)
282.5315877	0.0076	H-4->L+1 (35%), HOMO->L+19 (10%)
281.4860297	0.0081	H-3->L+2 (13%), HOMO->L+16 (18%), HOMO->L+18 (11%), HOMO->L+19 (10%)
281.122229	0.0082	H-3->L+3 (10%), HOMO->L+16 (22%), HOMO->L+19 (14%)
280.4735587	0.0113	H-1->L+9 (75%)
279.840507	0.0005	H-10->LUMO (13%), H-9->LUMO (23%), H-8->LUMO (19%)
279.4494481	0.0095	H-1->L+10 (76%)
277.7280065	0.0069	H-2->L+4 (10%), H-1->L+11 (36%)
277.0701185	0.0171	H-2->L+4 (35%), H-1->L+11 (15%)
276.8164876	0.0058	H-3->L+2 (27%)
276.3106163	0.0054	H-2->L+5 (61%)
274.3540454	0.0671	H-2->L+4 (12%), H-2->L+6 (14%), HOMO->L+16 (23%), HOMO->L+18 (14%)
272.2216196	0.0104	H-2->L+6 (45%), H-1->L+12 (24%)
271.0136763	0.0015	H-2->L+8 (47%)
270.4874591	0.0569	H-3->L+3 (13%), H-2->L+6 (11%), H-1->L+12 (20%), H-1->L+13 (10%)
269.9338935	0.1116	H-3->L+3 (20%), H-3->L+8 (10%), H-1->L+12 (22%)
268.9151646	0.0007	H-3->L+2 (13%), H-3->L+4 (50%)
267.9330437	0.0064	H-7->L+1 (14%), H-5->L+1 (12%), H-1->L+14 (21%)
266.5276595	0.0419	H-6->LUMO (15%), H-2->L+6 (14%), H-1->L+13 (47%)
265.7222329	0.0055	H-6->LUMO (56%), H-1->L+13 (14%)
264.4695747	0.0607	H-4->L+2 (48%), H-2->L+7 (10%)
263.8897828	0.0017	H-7->LUMO (13%), H-1->L+15 (27%)
263.5756216	0.0109	H-11->LUMO (17%), H-7->LUMO (13%), H-1->L+15 (16%)

263.2286717	0.0089	H-4->L+3 (19%), H-2->L+7 (14%), H-1->L+14 (23%)
263.1672114	0.0143	H-2->L+7 (18%), H-1->L+14 (32%)
262.9328088	0.0128	H-4->L+3 (14%), H-2->L+7 (36%)
262.5097113	0.0064	H-20->LUMO (13%), H-14->LUMO (23%), H-4->L+3 (30%)
261.617895	0.0052	H-3->L+5 (67%)
259.7760945	0.0003	H-4->L+2 (10%), H-4->L+4 (53%)
259.2437776	0.0003	H-3->L+6 (58%)
259.162493	0.0014	H-2->L+9 (74%)
258.7352337	0.0211	H-5->L+1 (10%), H-1->L+17 (49%)
258.3632088	0.0124	H-2->L+10 (59%)
257.9976208	0.0184	H-14->L+1 (16%), H-9->L+1 (13%)
257.6651911	0.1653	H-1->L+16 (18%), HOMO->L+20 (33%)
255.2305343	0.0177	H-4->L+5 (15%), H-2->L+10 (12%), H-2->L+11 (14%), H-1->L+16 (21%)
255.0310329	0.019	H-4->L+5 (28%), H-2->L+11 (14%), H-1->L+16 (20%)
254.8789915	0.0248	H-4->L+5 (30%), H-2->L+11 (48%)
253.3426033	0.2751	H-6->L+1 (57%)
252.2498762	0.0005	H-3->L+6 (14%), H-3->L+7 (20%), H-3->L+12 (10%)
252.0140184	0.0986	H-4->L+6 (27%), H-3->L+7 (12%)
251.7121501	0.0726	H-1->L+19 (11%)
251.6508416	0.0283	H-11->LUMO (17%), H-9->LUMO (13%), H-8->LUMO (17%), H-4->L+6 (21%)
251.5283142	0.0062	H-9->LUMO (10%), H-8->LUMO (23%), H-7->LUMO (10%), H-3->L+7 (24%)
251.2530633	0.0108	H-8->LUMO (12%), H-3->L+7 (27%)
251.2021571	0.0513	H-4->L+6 (13%), H-2->L+12 (44%)
249.6794745	0.0526	H-2->L+12 (12%), H-1->L+15 (10%), H-1->L+18 (26%)
248.7028337	0.0118	H-12->LUMO (76%)
248.2546487	0.0114	H-10->LUMO (26%), H-1->L+15 (15%)
247.8873493	0.0021	H-4->L+8 (28%), H-1->L+19 (29%)
247.2693736	0.0111	H-8->L+1 (17%), H-3->L+11 (19%), H-2->L+13 (14%)
246.7722954	0.0095	H-20->LUMO (12%), H-19->LUMO (10%), H-14->LUMO (19%), H-13->LUMO (10%), H-2->L+13 (19%)
246.6201274	0.0292	H-2->L+13 (38%)

246.1256534	0.007	H-13->LUMO (52%)
246.0133275	0.0184	H-13->LUMO (11%), H-3->L+9 (22%), H-3->L+11 (23%)