Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Table S1a. Bond Lengths for {[RuL^1(H_2O)(PPh_3)][PF_6]}·CH_2Cl_2.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ru1	P1	2.3409(16)	C20	C21	1.396(11)
Ru1	O1	2.008(4)	C21	C22	1.381(10)
Ru1	O2	2.006(5)	C23	C24	1.396(9)
Ru1	O3	2.185(5)	C23	C28	1.387(9)
Ru1	N1	2.003(5)	C24	C25	1.390(11)
Ru1	N2	1.983(5)	C25	C26	1.373(11)
P1	C17	1.819(7)	C26	C27	1.387(10)
P1	C23	1.819(7)	C27	C28	1.374(10)
P1	C29	1.825(6)	C29	C30	1.390(9)
O1	C12	1.324(8)	C29	C34	1.400(9)
O2	C1	1.328(8)	C30	C31	1.383(10)
N1	C7	1.297(9)	C31	C32	1.369(11)
N1	C8	1.482(9)	C32	C33	1.399(11)
N2	C9	1.478(8)	C33	C34	1.361(10)
N2	C10	1.296(9)	P2A	F1A	1.575(12)
C1	C2	1.419(10)	P2A	F2A	1.559(12)
C1	C6	1.405(10)	P2A	F3A	1.599(11)
C2	C3	1.417(10)	P2A	F4A	1.599(12)
C2	C7	1.433(11)	P2A	F5A	1.595(11)
C3	C4	1.362(12)	P2A	F6A	1.634(12)
C4	C5	1.406(13)	P2B	F1B	1.582(13)
C5	C6	1.357(11)	P2B	F2B	1.583(14)
C8	C9	1.524(10)	P2B	F3B	1.592(13)
C10	C11	1.432(10)	P2B	F4B	1.595(14)
C11	C12	1.417(10)	P2B	F5B	1.589(13)
C11	C16	1.422(10)	P2B	F6B	1.635(13)
C12	C13	1.420(10)	P2C	F1C	1.578(12)
C13	C14	1.370(10)	P2C	F2C	1.586(13)
C14	C15	1.402(12)	P2C	F3C	1.595(12)

C15	C16	1.365(11)	P2C	F4C	1.585(13)
C17	C18	1.402(9)	P2C	F5C	1.598(12)
C17	C22	1.404(10)	P2C	F6C	1.643(12)
C18	C19	1.396(10)	C41	Cl1	1.755(10)
C19	C20	1.380(11)	C41	Cl2	1.764(10)

Table S1b. Bond Angles for {[RuL^1(H$_2$O)(PPh$_3$)][PF$_6$]}·CH$_2$Cl$_2$.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	Ru1	P1	90.62(14)	C28	C23	P1	119.8(5)
O1	Ru1	O3	87.65(19)	C28	C23	C24	118.9(6)
O2	Ru1	P1	94.13(13)	C25	C24	C23	119.4(7)
O2	Ru1	O1	94.79(19)	C26	C25	C24	120.7(7)
O2	Ru1	O3	84.04(18)	C25	C26	C27	120.3(7)
O3	Ru1	P1	177.37(14)	C28	C27	C26	119.2(6)
N1	Ru1	P1	91.37(16)	C27	C28	C23	121.5(6)
N1	Ru1	O1	174.3(2)	C30	C29	P1	125.2(5)
N1	Ru1	O2	90.3(2)	C30	C29	C34	118.5(6)
N1	Ru1	O3	90.5(2)	C34	C29	P1	116.3(5)
N2	Ru1	P1	95.07(15)	C31	C30	C29	119.8(6)
N2	Ru1	O1	91.7(2)	C32	C31	C30	120.9(7)
N2	Ru1	O2	168.69(19)	C31	C32	C33	119.9(7)
N2	Ru1	O3	87.0(2)	C34	C33	C32	119.3(7)
N2	Ru1	N1	82.9(2)	C33	C34	C29	121.5(7)
C17	P1	Ru1	114.1(2)	F1A	P2A	F3A	89.1(9)
C17	P1	C29	107.6(3)	F1A	P2A	F4A	89.8(10)
C23	P1	Ru1	116.4(2)	F1A	P2A	F5A	89.2(9)
C23	P1	C17	103.6(3)	F1A	P2A	F6A	178.0(11)
C23	P1	C29	101.9(3)	F2A	P2A	F1A	93.5(10)
C29	P1	Ru1	112.1(2)	F2A	P2A	F3A	90.9(10)
C12	O1	Ru1	123.2(4)	F2A	P2A	F4A	176.3(12)

C1	O2	Ru1	125.1(4)	F2A	P2A	F5A	91.1(10)
C7	N1	Ru1	126.1(5)	F2A	P2A	F6A	88.3(10)
C7	N1	C8	120.8(6)	F3A	P2A	F4A	87.5(9)
C8	N1	Ru1	113.0(4)	F3A	P2A	F6A	91.7(9)
C9	N2	Ru1	113.2(4)	F4A	P2A	F6A	88.4(10)
C10	N2	Ru1	125.6(5)	F5A	P2A	F3A	177.5(12)
C10	N2	C9	120.9(6)	F5A	P2A	F4A	90.5(9)
O2	C1	C2	123.4(6)	F5A	P2A	F6A	89.8(9)
O2	C1	C6	118.7(6)	F1B	P2B	F2B	89.6(11)
C6	C1	C2	117.9(7)	F1B	P2B	F3B	93.4(11)
C1	C2	C7	124.4(6)	F1B	P2B	F4B	93.3(11)
C3	C2	C1	118.5(7)	F1B	P2B	F5B	88.5(10)
C3	C2	C7	117.0(7)	F1B	P2B	F6B	176.2(13)
C4	C3	C2	122.3(8)	F2B	P2B	F3B	88.5(11)
C3	C4	C5	118.3(8)	F2B	P2B	F4B	175.8(14)
C6	C5	C4	121.0(8)	F2B	P2B	F5B	91.5(12)
C5	C6	C1	121.9(8)	F2B	P2B	F6B	88.7(11)
N1	C7	C2	125.4(6)	F3B	P2B	F4B	88.3(12)
N1	C8	C9	108.6(5)	F3B	P2B	F6B	89.9(11)
N2	C9	C8	107.7(5)	F4B	P2B	F6B	88.5(11)
N2	C10	C11	124.5(6)	F5B	P2B	F3B	178.1(13)
C12	C11	C10	125.4(6)	F5B	P2B	F4B	91.6(12)
C12	C11	C16	118.3(6)	F5B	P2B	F6B	88.1(11)
C16	C11	C10	116.2(6)	F1C	P2C	F2C	90.1(10)
O1	C12	C11	124.3(6)	F1C	P2C	F3C	90.5(10)
O1	C12	C13	117.2(6)	F1C	P2C	F4C	93.2(10)
C11	C12	C13	118.4(6)	F1C	P2C	F5C	92.6(10)
C14	C13	C12	120.9(7)	F1C	P2C	F6C	177.8(12)

C13	C14	C15	121.3(7)	F2C	P2C	F3C	92.9(10)
C16	C15	C14	118.6(7)	F2C	P2C	F5C	88.8(10)
C15	C16	C11	122.4(7)	F2C	P2C	F6C	87.9(10)
C18	C17	P1	120.9(5)	F3C	P2C	F5C	176.5(11)
C18	C17	C22	118.6(6)	F3C	P2C	F6C	90.6(9)
C22	C17	P1	120.1(5)	F4C	P2C	F2C	176.6(11)
C19	C18	C17	120.2(7)	F4C	P2C	F3C	87.2(10)
C20	C19	C18	120.3(7)	F4C	P2C	F5C	90.9(10)
C19	C20	C21	120.1(7)	F4C	P2C	F6C	88.7(10)
C22	C21	C20	119.9(7)	F5C	P2C	F6C	86.4(10)
C21	C22	C17	120.9(7)	Cl1	C41	Cl2	112.9(11)
C24	C23	P1	121.0(5)				

Table S1c. Torsion Angles for {[RuL^1(H$_2$O)(PPh$_3$)][PF$_6$]}·CH$_2$Cl$_2$.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Ru1	P1	C17	C18	-67.0(6)	C10	C11	C12	O1	-1.9(10)
Ru1	P1	C17	C22	105.3(5)	C10	C11	C12	C13	-178.4(6)
Ru1	P1	C23	C24	-22.2(6)	C10	C11	C16	C15	178.8(6)
Ru1	P1	C23	C28	163.3(5)	C11	C12	C13	C14	0.0(10)
Ru1	P1	C29	C30	119.9(5)	C12	C11	C16	C15	0.7(10)
Ru1	P1	C29	C34	-59.9(5)	C12	C13	C14	C15	0.2(11)
Ru1	O1	C12	C11	20.0(9)	C13	C14	C15	C16	0.0(11)
Ru1	O1	C12	C13	-163.5(5)	C14	C15	C16	C11	-0.5(11)
Ru1	O2	C1	C2	22.5(9)	C16	C11	C12	O1	176.0(6)
Ru1	O2	C1	C6	-159.2(5)	C16	C11	C12	C13	-0.5(9)
Ru1	N1	C7	C2	-0.2(9)	C17	P1	C23	C24	103.9(6)
Ru1	N1	C8	C9	-29.8(6)	C17	P1	C23	C28	-70.6(6)
Ru1	N2	C9	C8	-35.3(6)	C17	P1	C29	C30	-6.4(7)
Ru1	N2	C10	C11	-9.3(9)	C17	P1	C29	C34	173.8(5)

P1	C17	C18	C19	171.5(5)	C17	C18	C19	C20	0.1(10)
P1	C17	C22	C21	-171.3(6)	C18	C17	C22	C21	1.2(10)
P1	C23	C24	C25	-173.5(6)	C18	C19	C20	C21	0.5(11)
P1	C23	C28	C27	174.8(5)	C19	C20	C21	C22	-0.2(12)
P1	C29	C30	C31	-179.0(5)	C20	C21	C22	C17	-0.6(11)
P1	C29	C34	C33	179.6(5)	C22	C17	C18	C19	-0.9(10)
O1	C12	C13	C14	-176.7(6)	C23	P1	C17	C18	165.5(5)
O2	C1	C2	C3	176.6(6)	C23	P1	C17	C22	-22.2(6)
O2	C1	C2	C7	-1.4(11)	C23	P1	C29	C30	-115.0(6)
O2	C1	C6	C5	-177.3(7)	C23	P1	C29	C34	65.2(5)
N1	C8	C9	N2	41.1(7)	C23	C24	C25	C26	-1.5(12)
N2	C10	C11	C12	-4.3(11)	C24	C23	C28	C27	0.2(10)
N2	C10	C11	C16	177.8(6)	C24	C25	C26	C27	0.9(13)
C1	C2	C3	C4	1.0(11)	C25	C26	C27	C28	0.3(11)
C1	C2	C7	N1	-10.7(11)	C26	C27	C28	C23	-0.9(11)
C2	C1	C6	C5	1.1(11)	C28	C23	C24	C25	1.0(11)
C2	C3	C4	C5	0.5(12)	C29	P1	C17	C18	58.0(6)
C3	C2	C7	N1	171.3(6)	C29	P1	C17	C22	-129.6(5)
C3	C4	C5	C6	-1.3(13)	C29	P1	C23	C24	-144.5(6)
C4	C5	C6	C1	0.4(12)	C29	P1	C23	C28	41.0(6)
C6	C1	C2	C3	-1.8(10)	C29	C30	C31	C32	-0.6(11)
C6	C1	C2	C7	-179.7(6)	C30	C29	C34	C33	-0.2(10)
C7	N1	C8	C9	153.7(6)	C30	C31	C32	C33	-0.2(11)
C7	C2	C3	C4	179.1(7)	C31	C32	C33	C34	0.8(11)
C8	N1	C7	C2	175.8(6)	C32	C33	C34	C29	-0.6(10)
C9	N2	C10	C11	176.5(6)	C34	C29	C30	C31	0.8(10)
C10	N2	C9	C8	139.5(6)					

Table S1d. The optimized geometrical data of $[RuL^1(H_2O)(PPh_3)]$ and $[RuL^1(H_2O)(PPh_3)]^+$ at gaseous state

B3LYP/DGDZVP					
Bond length of ligand and complex (Å)					
Atoms		**Experimental**		**Gaseous state**	
	L^1		**$[RuL^1(H_2O)(PPh_3)]^+$**	**$[RuL^1(H_2O)(PPh_3)]^+$**	**$[RuL^1(H_2O)(PPh_3)]$**
C1-C2	1.433	Ru1-$N1_{imine}$	2.003(5)	2.059	2.358
C1-C7	1.456	Ru1-$N2_{imine}$	1.983(5)	2.040	2.321
C7-$N1_{imine}$	1.301	Ru1-O2	2.341(16)	2.049	2.148
$N1_{imine}$-C8	1.457	Ru1-O1	2.006(5)	2.046	2.151
C8-C9	1.546	Ru1-H_2O	2.185(5)	2.325	3.370
C9-$N2_{imine}$	1.455	Ru1-P1	2.341(16)	2.384	2.650
$N2_{imine}$-C10	1.291	**Bond Angle (°)**			
C10-C11	1.475	$N1_{imine}$-Ru1-$N2_{imine}$	82.9(2)	81.99	72.53
C11-C12	1.420	$N1_{imine}$-Ru1-O1	174.30(2)	171.50	139.47
O1-C2	1.351	$N1_{imine}$-Ru1-O2	90.30(2)	88.29	79.37
O2-C12	1.380	$N1_{imine}$-Ru1-H_2O	90.50(2)	88.86	136.42
O1-H	1.029	$N1_{imine}$-Ru1-P1	91.37(16)	94.90	107.91
O2-H	0.978	$N2_{imine}$-Ru1-O2	168.69(19)	163.79	149.66
		$N2_{imine}$-Ru1-O1	91.7(2)	90.12	79.90
		$N2_{imine}$-Ru1-H_2O	87.0(2)	87.84	140.16
		$N2_{imine}$-Ru1-P1	95.07(15)	98.68	97.34
		O2-Ru1-O1	87.65(19)	98.65	116.78
		O2-Ru1- H_2O	87.65(19)	78.99	60.25
		O1-Ru1-H_2O	87.65(19)	87.68	60.50
		O2-Ru1-P1	87.65(19)	95.03	102.02
		O1-Ru1-P1	90.62(14)	89.40	104.53
		H_2O-Ru1-P1	177.37(14)	172.86	96.57
		Methanol			
C1-C2	1.433	Ru1-$N1_{imine}$	2.003(5)	2.055	2.043
C1-C7	1.458	Ru1-$N2_{imine}$	1.983(5)	2.038	2.037
C7-$N1_{imine}$	1.301	Ru1-O2	2.341(16)	2.05	2.147
$N1_{imine}$-C8	1.459	Ru1-O1	2.006(5)	2.055	2.143

C8-C9	1.543	Ru1-H_2O	2.185(5)	2.303	2.321
C9-$N2_{imine}$	1.459	Ru1-P1	2.341(16)	2.389	2.330
$N2_{imine}$-C10	1.293	**Bond Angle (°)**			
C10-C11	1.475	$N1_{imine}$-Ru1-$N2_{imine}$	82.9(2)	82.08	83.27
C11-C12	1.422	$N1_{imine}$-Ru1-O1	174.3(2)	171.69	166.76
O1-C2	1.356	$N1_{imine}$-Ru1-O2	90.3(2)	88.65	89.81
O2-C12	1.378	$N1_{imine}$-Ru1-H_2O	90.5(2)	87.57	87.92
O1-H	1.040	$N1_{imine}$-Ru1-P1	91.37(16)	94.88	97.54
O2-H	0.980	$N2_{imine}$-Ru1-O2	168.69(19)	164.75	168.17
H-O1-$N1_{imine}$	1.611	$N2_{imine}$-Ru1-O1	91.7(2)	90.17	90.401
		$N2_{imine}$-Ru1-H_2O	87.0(2)	86.92	91.96
		$N2_{imine}$-Ru1-P1	95.07(15)	98.41	96.62
		O2-Ru1-O1	87.65(19)	98.28	94.34
		O2-Ru1-H_2O	87.65(19)	80.59	78.16
		O1-Ru1-H_2O	87.65(19)	89.03	80.66
		O2-Ru1-P1	87.65(19)	94.40	93.79
		O1-Ru1-P1	90.62(14)	89.19	94.73
		H_2O-Ru1-P1	177.37(14)	174.38	170.30

Table S2a. $M-N_{imine}$ bond distance for different trivalent transition metal ions with salen ligands.

Metal	M-N	Ref.
$Mn^{3+}(d^4)$	2.292	[1, 2]
$Fe^{3+}(d^5)$	2.111	[3]
$Ru^{3+}(d^5)$	2.011	[4-6]
$Ru^{3+}(d^5)$	2.003	this work
$Co^{3+}(d^6)$	1.953	[7, 8]

Table S2b. Bond length (M-Nimine) of different divalent metal ions.

Metal ions	M-N	Ref
$Mn^{2+}(d^5)$	2.239	[9], [10]
$Fe^{2+}(d^6)$	2.226	[11]
$Ru^{2+}(d^6)$	2.071	[12], [13]
$Co^{2+}(d^7)$	2.119	[14], [10]
$Ni^{2+}(d^8)$	2.055	[15], [10]
$Cu^{2+}(d^9)$	1.956	[16], [15]
$Zn^{2+}(d^{10})$	1.985	[17], [10]

Note: All references are in last page.

Table S3. The optimized geometrical data of $[RuL^1(H_2O)(AcO)]$ and $[RuL^1(AcO)(PPh_3)]$ at gaseous state and methanol

B3LYP/DGDZVP					
Bond length of ligand and complex (Å)					
Atoms		**Experimental**		**Gaseous state**	
	(L^1)		**$[RuL^1(H_2O)(PPh_3)]^+$**	**$[RuL^1(H_2O)(AcO)]$**	**$[RuL^1(AcO)(PPh_3)]$**
C1-C2	1.433	Ru1-$N1_{imine}$	2.003(5)	2.002	2.034
C1-C7	1.456	Ru1-$N2_{imine}$	1.983(5)	1.990	2.023
C7-$N1_{imine}$	1.301	Ru1-O2	2.341(16)	2.035	2.079
$N1_{imine}$-C8	1.457	Ru1-O1	2.006(5)	2.025	2.067
C8-C9	1.546	Ru1-H_2O	2.185(5)	2.271	-
C9-$N2_{imine}$	1.455	Ru1-P1	2.341(16)	-	2.474
$N2_{imine}$-C10	1.291	Ru-AcO	-	1.985	2.092
C11-C12	1.420	**Bond Angle (°)**			
O1-C2	1.351	$N1_{imine}$-Ru1-$N2_{imine}$	82.9(2)	84.05	83.03
O2-C12	1.380	$N1_{imine}$-Ru1-O1	174.30(2)	170.36	173.18
O1-H	1.029	$N1_{imine}$-Ru1-O2	90.30(2)	91.44	90.95
O2-H	0.978	$N1_{imine}$-Ru1-H_2O	90.50(2)	89.10	-
H-O1-$N1_{imine}$	1.652	$N1_{imine}$-Ru1-P1	91.37(16)	-	93.73
		$N1_{imine}$-Ru1-AcO	-	97.9	92.76
		$N2_{imine}$-Ru1-O2	168.69(19)	175.26	172.29
		$N2_{imine}$-Ru1-O1	91.7(2)	90.41	90.16
		$N2_{imine}$-Ru1-H_2O	87.0(2)	91.18	-
		$N2_{imine}$-Ru1-P1	95.07(15)	-	97.69
		$N2_{imine}$-Ru1-AcO	-	93.19	90.77
		O2-Ru1-O1	87.65(19)	93.85	95.80
		O2-Ru1-H_2O	87.65(19)	87.28	-
		O1-Ru1-H_2O	87.65(19)	83.11	-
		O2-Ru1-P1	87.65(19)	-	87.47
		$O1_{imine}$-Ru1-AcO	-	90.23	86.93
		O1-Ru1-P1	90.62(14)	-	87.54
		H_2O-Ru1-P1	177.37(14)	-	-

		$O2_{imine}$-Ru1-AcO	-	88.87	84.69
		Methanol			
C1-C2	1.433	Ru1-$N1_{imine}$	2.003(5)	2.332	2.036
C1-C7	1.458	Ru1-$N2_{imine}$	1.983(5)	2.305	2.024
C7-$N1_{imine}$	1.301	Ru1-O2	2.341(16)	2.136	2.081
$N1_{imine}$-C8	1.459	Ru1-O1	2.006(5)	2.169	2.070
C8-C9	1.543	Ru1-H_2O	2.185(5)	2.575	-
C9-$N2_{imine}$	1.459	Ru1-P1	2.341(16)	-	2.465
$N2_{imine}$-C10	1.293	Ru-AcO	-	2.198	2.138
C10-C11	1.475				
C11-C12	1.422	**Bond Angle (°)**	-		
O1-C2	1.356	$N1_{imine}$-Ru1-$N2_{imine}$	82.9(2)	73.02	82.90
O2-C12	1.378	$N1_{imine}$-Ru1-O1	174.3(2)	134.78	173.07
O1-H	1.040	$N1_{imine}$-Ru1-O2	90.3(2)	80.22	90.54
O2-H	0.980	$N1_{imine}$-Ru1-H_2O	90.5(2)	92.04	-
H-O1-$N1_{imine}$	1.611	$N1_{imine}$-Ru1-P1	91.37(16)		93.40
		$N1_{imine}$-Ru1-AcO	-	126.43	93.60
		$N2_{imine}$-Ru1-O2	168.69(19)	151.18	171.26
		$N2_{imine}$-Ru1-O1	91.7(2)	79.38	90.20
		$N2_{imine}$-Ru1-H_2O	87.0(2)	114.93	-
		$N2_{imine}$-Ru1-P1	95.07(15)	-	97.07
		$N2_{imine}$-Ru1-AcO	-	91.06	91.06
		O2-Ru1-O1	87.65(19)	128.46	96.25
		O2-Ru1-H_2O	87.65(19)	75.94	-
		O1-Ru1-H_2O	87.65(19)	68.04	-
		O2-Ru1-P1	87.65(19)	-	89.05
		O1-Ru1-P1	90.62(14)	-	88.08
		$O1_{imine}$-Ru1-AcO	-	88.49	85.83
		H_2O-Ru1-P1	177.37(14)	-	-
		H_2O-Ru1-AcO	-	139.42	-
		$O2_{imine}$-Ru1-AcO	-	96.41	83.57

Table S4. TDDFT spectral data of electronic transitions $[RuL^1(H_2O)(PPh_3)]$, $[RuL^1(H_2O)(PPh_3)]^+$, $[RuL^1(H_2O)(AcO)]$ and $[RuL^1(AcO)(PPh_3)]$ at gaseous state and methanol, L^1= N, N′-Bis (salicylidene)ethylenediamine with oscillator strength f > 0.0001.

Wevelength (nm)	Osc. Strength (f)	Contribution percentage	Character	Theory (nm)	Experimental (nm)
		Gaseous state			
		$[RuL^1(H_2O)(PPh_3)]$			
1289.62	0.0003	HOMO->LUMO+1 (46%) HOMO->LUMO+2 (35%) HOMO-2->LUMO+1 (4%) HOMO-2->LUMO+2 (3%) HOMO->LUMO+4 (3%) HOMO-1->LUMO+2 (2%)	MLCT		
876.03	0.0009	HOMO->LUMO+2 (44%) HOMO->LUMO+1 (38%) HOMO-2->LUMO+1 (3%) HOMO-2->LUMO+2 (3%) HOMO-1->LUMO+2 (3%) HOMO-1->LUMO+1 (2%)	MLCT	902	
559.70	0.0003	HOMO->LUMO+8 (49%) HOMO->LUMO (14%) HOMO->LUMO+4 (7%) HOMO->LUMO+10 (4%) HOMO-2->LUMO+8 (4%) HOMO-1->LUMO+8 (3%) HOMO->LUMO+7 (3%) HOMO->LUMO+9 (3%)	MLCT		
541.87	0.0634	HOMO-1->LUMO (53%) HOMO-2->LUMO (29%) HOMO->LUMO (10%) HOMO->LUMO+8 (2%)	MLCT	545	

536.77	0.0134	HOMO-2->LUMO (52%) HOMO-1->LUMO (30%) HOMO->LUMO (7%) HOMO->LUMO+1 (2%) HOMO->LUMO+3 (2%)	MLCT
526.32	0.0039	HOMO->LUMO (70%) HOMO->LUMO+8 (8%) HOMO-1->LUMO (4%) HOMO-2->LUMO (3%) HOMO->LUMO+4 (2%)	MLCT
501.62	0.0053	HOMO->LUMO+1 (84%) HOMO-2->LUMO (3%) HOMO-1->LUMO (3%) HOMO-1->LUMO (2%)	MLCT
477.71	0.001	HOMO-1->LUMO (47%) HOMO-2->LUMO+3 (13%) HOMO-2->LUMO (11%) HOMO-2->LUMO+1 (5%) HOMO->LUMO+1 (4%) HOMO-2->LUMO+1 (4%) HOMO->LUMO+3 (3%) HOMO-3->LUMO (2%)	MLCT
471.66	0.0002	HOMO-1->LUMO+1 (38%) HOMO-1->LUMO+1 (20%) HOMO-2->LUMO+1 (12%) HOMO-1->LUMO+4 (9%) HOMO-2->LUMO (6%) HOMO-2->LUMO+1 (3%) HOMO-1->LUMO+2 (2%)	MLCT
		$[RuL^1(H_2O)(PPh_3)]^+$	
1149.49	0.0003	HOMO-1->LUMO (93%) HOMO->LUMO (2%)	MLCT

1018.27	0.0866	HOMO->LUMO+1 (78%) HOMO->LUMO+2 (14%) HOMO-2->LUMO+1 (2%) HOMO->LUMO (2%)	MLCT		
960.97	0.0254	HOMO->LUMO+2 (79%) HOMO->LUMO+1 (14%) HOMO-1->LUMO+1 (3%)	MLCT		915
836.71	0.0013	HOMO-1->LUMO+2 (81%) HOMO-1->LUMO+1 (12%)	MLCT	808	
780.51	0.0345	HOMO-1->LUMO+1 (62%) HOMO-2->LUMO (13%) HOMO-1->LUMO+2 (13%) HOMO-6->LUMO (2%)	MLCT		740
709.74	0.0079	HOMO-2->LUMO (70%) HOMO-1->LUMO+1 (9%) HOMO-2->LUMO+2 (8%) HOMO->LUMO+2 (3%) HOMO-12->LUMO (2%)	MLCT		
639.32	0.0052	HOMO-2->LUMO+1 (91%) HOMO-12->LUMO+1 (3%) HOMO->LUMO+1 (2%)	MLCT	630	
567.04	0.0332	HOMO-2->LUMO+2 (48%) HOMO-3->LUMO (20%) HOMO-4->LUMO (7%) HOMO-2->LUMO (6%) HOMO-6->LUMO (4%) HOMO-5->LUMO (4%) HOMO-12->LUMO+2 (2%)	MLCT		497
555.73	0.0339	HOMO-3->LUMO (29%) HOMO-2->LUMO+2 (25%) HOMO-5->LUMO (16%)	MLCT	495	343

		HOMO-4->LUMO (14%) HOMO-10->LUMO+1 (3%) HOMO-6->LUMO (2%)		
		[RuL^1(H$_2$O)(AcO)]		
1923.43	0. 0004	HOMO-1->LUMO (66%) HOMO-3->LUMO (19%) HOMO->LUMO (8%) HOMO-4->LUMO (5%)	MLCT	
1493.97	0.0003	HOMO-3->LUMO (66%) HOMO-1->LUMO (17%) HOMO-2->LUMO (13%) HOMO-6->LUMO (4%)	MLCT	
861.90	0.1422	HOMO->LUMO (65%) HOMO-4->LUMO (23%) HOMO-1->LUMO (14%)	MLCT	
724.71	0.153	HOMO-4->LUMO (57%) HOMO->LUMO (28%) HOMO-2->LUMO (9%) HOMO-6->LUMO (3%) HOMO-3->LUMO (2%)	MLCT	758
681.79	0.0268	HOMO-2->LUMO (70%) HOMO-3->LUMO (12%) HOMO-4->LUMO (10%) HOMO-5->LUMO (3%)	MLCT	
554.99	0.0077	HOMO-5->LUMO (92%) HOMO-6->LUMO (2%)	MLCT	534
523.03	0.024	HOMO-6->LUMO (87%) HOMO-1->LUMO (3%) HOMO-4->LUMO (3%) HOMO-5->LUMO (2%)	MLCT	
432.51	0.0015	HOMO-9->LUMO (16%)	MLCT	

		HOMO-8->LUMO (63%) HOMO-10->LUMO (7%) HOMO-7->LUMO (9%)		
423.08	0.0022	HOMO-1->LUMO+3 (54%) HOMO-7->LUMO (10%) HOMO-6->LUMO+3 (7%) HOMO-4->LUMO+3 (7%) HOMO->LUMO+3 (7%) HOMO-1->LUMO+2 (3%) HOMO-9->LUMO (2%) HOMO-8->LUMO (2%)	MLCT	427
414.16	0.0008	HOMO-9->LUMO (71%) HOMO-8->LUMO (25%)	MLCT	
		[RuL^1(AcO)(PPh$_3$)]		
2665.75	0.0006	HOMO-1->LUMO (43%) HOMO->LUMO (41%) HOMO-3->LUMO (5%) HOMO-2->LUMO (5%) HOMO-4->LUMO (2%)	MLCT	
1517.55	0.0001	HOMO-2->LUMO (81%) HOMO-4->LUMO (8%) HOMO->LUMO (3%)	MLCT	
805.46	0.0825	HOMO->LUMO (52%) HOMO-1->LUMO (43%)	MLCT	802
678.29	0.0094	HOMO-3->LUMO (81%) HOMO-1->LUMO (8%) HOMO-4->LUMO (4%)	MLCT	
589.14	0.0068	HOMO-4->LUMO (80%) HOMO-2->LUMO (8%) HOMO-3->LUMO (6%)	MLCT	606

		HOMO-1->LUMO (2%)		
493.528	0.003	HOMO->LUMO+1 (28%) HOMO->LUMO+2 (18%) HOMO-5->LUMO (17%) HOMO->LUMO (11%) HOMO->LUMO+1 (9%) HOMO-1->LUMO+1 (5%)	MLCT	
485.68	0.0006	HOMO-5->LUMO (60%) HOMO->LUMO (16%) HOMO-6->LUMO (4%) HOMO->LUMO+2 (4%) HOMO-1->LUMO+1 (3%) HOMO-1->LUMO (2%)	MLCT	
475.65	0.0078	HOMO->LUMO (26%) HOMO-1->LUMO (14%) HOMO-5->LUMO (14%) HOMO->LUMO+1 (13%) HOMO->LUMO+1 (8%) HOMO-1->LUMO+1 (6%) HOMO-2->LUMO+1 (2%) HOMO-1->LUMO+2 (2%)	MLCT	478
453.80	0.0001	HOMO->LUMO+2 (52%) HOMO->LUMO+8 (7%) HOMO-5->LUMO+2 (4%) HOMO->LUMO+3 (4%) HOMO-1->LUMO+3 (3%) HOMO->LUMO+4 (3%) HOMO-5->LUMO+8 (2%) HOMO->LUMO+6 (2%)	MLCT	
		Methanol		
		$[RuL^1(H_2O)(PPh_3)]$		

536.66	0.016	HOMO->LUMO+1 (18%) HOMO->LUMO+2 (54%) HOMO-4->LUMO+2 (3%) HOMO->LUMO+4 (4%) HOMO->LUMO+8 (9%) HOMO->LUMO+10 (2%)	MLCT	
483.20	0.016	HOMO->LUMO (88%) HOMO-1->LUMO+2 (4%)	MLCT	496
474.76	0.0034	HOMO-1->LUMO+1 (34%) HOMO-1->LUMO+2 (32%) HOMO->LUMO+1 (10%) HOMO-1->LUMO+8 (6%) HOMO->LUMO (6%) HOMO-1->LUMO+10 (3%)	MLCT	
459.78	0.0332	HOMO-1->LUMO+2 (10%) HOMO->LUMO+1 (63%) HOMO->LUMO+2 (18%)	MLCT	
445.62	0.0117	HOMO-1->LUMO (93%) HOMO->LUMO (3%)	MLCT	
436.38	0.0011	HOMO-2->LUMO+2 (43%) HOMO-1->LUMO+1 (12%) HOMO-2->LUMO+8 (9%) HOMO-2->LUMO+1 (8%) HOMO-3->LUMO+2 (6%) HOMO-2->LUMO+4 (3%)	MLCT	
429.44	0.003	HOMO-1->LUMO+1 (46%) HOMO-1->LUMO+2 (29%) HOMO-2->LUMO+2 (7%) HOMO-2->LUMO+1 (4%)	MLCT	
384.09	0.0012	HOMO->LUMO+3 (92%) HOMO->LUMO+4 (5%)	MLCT	395

379.30	0.0153	HOMO->LUMO+4 (78%) HOMO->LUMO+3 (7%) HOMO->LUMO+2 (6%)	MLCT	
373.56	0.2449	HOMO-2->LUMO (79%) HOMO-3->LUMO (8%) HOMO-1->LUMO+11 (5%) HOMO->LUMO+4 (2%)	MLCT	
		$[RuL^1(H_2O)(PPh_3)]^+$		
1333.59	0.002	HOMO->LUMO (96%) HOMO-1->LUMO (2%)	MLCT	1134
1124.37	0.0014	HOMO-1->LUMO (94%) HOMO->LUMO (2%)	MLCT	
955.56	0.1331	HOMO->LUMO+1 (93%)	MLCT	
888.33	0.0038	HOMO->LUMO+2 (93%) HOMO-1->LUMO+1 (2%)	MLCT	
780.02	0.0023	HOMO-1->LUMO+2 (82%) HOMO-1->LUMO+1 (12%)	MLCT	
761.81	0.0435	HOMO-1->LUMO+1 (68%) HOMO-2->LUMO (10%) HOMO-1->LUMO+2 (13%)	MLCT	
681.79	0.0117	HOMO-2->LUMO (76%) HOMO-1->LUMO+1 (7%) HOMO-2->LUMO+2 (5%) HOMO-12->LUMO (2%) HOMO->LUMO+2 (2%)	MLCT	
599.01	0.0049	HOMO-2->LUMO+1 (93%) HOMO-12->LUMO+1 (3%)	MLCT	602

555.76	0.0261	HOMO-3->LUMO (76%) HOMO-2->LUMO+2 (8%) HOMO-10->LUMO (8%) HOMO-6->LUMO (2%)	MLCT	
541.01	0.0384	HOMO-2->LUMO+2 (63%) HOMO-3->LUMO (11%) HOMO-4->LUMO (10%) HOMO-10->LUMO+1 (3%) HOMO-6->LUMO (3%) HOMO-12->LUMO+2 (2%)	MLCT	
		[RuL^1(H_2O)(AcO)]		
965.99	0.0077	HOMO->LUMO (67%) HOMO-1->LUMO (27%) HOMO->LUMO+1 (3%) HOMO-1->LUMO+1 (2%)	MLCT	984
912.59	0.0438	HOMO-1->LUMO (59%) HOMO->LUMO (29%) HOMO-1->LUMO+1 (8%)	MLCT	
796.00	0.0485	HOMO->LUMO+1 (86%) HOMO-1->LUMO+2 (4%) HOMO-1->LUMO (3%) HOMO-1->LUMO+1 (2%)	MLCT	
756.19	0.0029	HOMO-1->LUMO+1 (82%) HOMO-1->LUMO (6%) HOMO->LUMO+1 (6%) HOMO-1->LUMO+2 (3%)	MLCT	
696.07	0.0016	HOMO-1->LUMO+2 (71%) HOMO->LUMO+2 (20%) HOMO-1->LUMO+1 (3%) HOMO->LUMO+1 (3%)	MLCT	

		HOMO-1->LUMO (2%)		
692.57	0.0225	HOMO->LUMO+2 (77%) HOMO-1->LUMO+2 (18%)	MLCT	
580.59	0.002	HOMO-2->LUMO (96%) HOMO-7->LUMO (2%)	MLCT	555
516.36	0.0078	HOMO-3->LUMO (56%) HOMO-5->LUMO (27%) HOMO-6->LUMO (6%) HOMO-4->LUMO (4%) HOMO-2->LUMO+1 (2%)	MLCT	
513.31	0.0014	HOMO-2->LUMO+1 (94%)	MLCT	
503.14	0.0084	HOMO-1->LUMO+3 (54%) HOMO->LUMO+3 (24%) HOMO-5->LUMO (6%) HOMO-3->LUMO (5%)	MLCT	
		[RuL^1(AcO)(PPh$_3$)]		
2657.75	0.0005	HOMO-1->LUMO (48%) HOMO->LUMO (37%) HOMO-3->LUMO (10%)	MLCT	
801.09	0.116	HOMO->LUMO (54%) HOMO-1->LUMO (29%) HOMO-2->LUMO (13%) HOMO-3->LUMO (2%)	MLCT	939
663.80	0.0126	HOMO-3->LUMO (79%) HOMO-1->LUMO (10%) HOMO-2->LUMO (2%) HOMO->LUMO (2%	MLCT	
514.93	0.003	HOMO-4->LUMO (91%)	MLCT	

		HOMO-3->LUMO (2%) HOMO-2->LUMO (2%)		
509.91	0.0002	HOMO-2->LUMO+2 (17%) HOMO-1->LUMO+3 (16%) HOMO->LUMO+3 (14%) HOMO->LUMo+2 (8%) HOMO-3->LUMO+3 (5%) HOMO-1->LUMO+9 (4%) HOMO-2->LUMO+8 (2%)	MLCT	506
486.77	0.0003	HOMO-5->LUMO (85%) HOMO->LUMO+1 (2%) HOMO-14->LUMO (2%) HOMO-10->LUMO (2%)	MLCT	
472.21	0.0034	HOMO->LUMO+1 (24%) HOMO->LUMO (22%) HOMO->LUMO+2 (19%) HOMO->LUMO+1 (8%) HOMO-1->LUMO+1 (7%) HOMO-6->LUMO (3%) HOMO-5->LUMO (2%)	MLCT	
462.92	0.0102	HOMO->LUMO (28%) HOMO->LUMO+1 (17%) HOMO-1->LUMO (13%) HOMO-2->LUMO+1 (5%) HOMO->LUMO+1 (5%) HOMO-5->LUMO (3%)	MLCT	
458.25	0.0001	HOMO-3->LUMO+2 (18%) HOMO-2->LUMO+3 (30%) HOMO-2->LUMO+9 (6%) HOMO-2->LUMO+2 (5%) HOMO-1->LUMO+3 (3%) HOMO-12->LUMO+2(2%) HOMO-10->LUMO+3 (2%)	MLCT	

HOMO-2->LUMO+7 (2%)

Table S5. Electronic properties of ligand (L^1) and ruthenium complexes at gaseous state and methanol

B3LYP/DGDZVP												
Gaseous state							**Methanol**					
Compounds	**E_{HF}**	**HOMO (eV)**	**LUMO (eV)**	**ΔE (eV)**	**Hardness (η, eV)**	**Softness (σ, eV)**	**E_{HF}**	**HOMO (eV)**	**LUMO (eV)**	**ΔE (eV)**	**Hardness (η, eV)**	**Softness (σ, eV)**
L^1	-879.26	-5.252	-2.320	2.932	1.466	0.682	-879.27	-5.585	-2.479	3.105	1.553	0.644
$[RuL^1(H_2O)(PPh_3)]^+$	-6433.65	-8.516	-6.252	2.264	1.132	0.884	-6433.71	-6.244	-3.961	2.283	1.142	0.876
$[RuL^1(H_2O)(PPh_3)]$	-6433.77	-5.422	-2.546	2.876	1.438	0.695	-6433.87	-4.888	-1.562	3.326	1.663	0.601
$[RuL^1(H_2O)(AcO)]$	5625.79	-9.277	-7.657	1.621	0.810	1.234	-5626.06	-6.098	-3.109	2.189	1.094	0.914
$[RuL^1(AcO)(PPh_3)]$	6585.69	-8.680	-7.233	1.447	0.724	1.382	-6585.75	-6.518	-5.062	1.456	0.728	1.373

Table S6. Condensed Mulliken charges of $[RuL^1(H_2O)(PPh_3)]$, $[RuL^1(H_2O)(PPh_3)]^+$, $[RuL^1(H_2O)(AcO)]$ and $[RuL^1(AcO)(PPh_3)]$ at gaseous state and methanol.

B3LYP/DGDZVP					
Bond length of Ligands (Å)					
	L^1	**$[RuL^1(H_2O)(PPh_3)]$**	**$[RuL^1(H_2O)(PPh_3)]^+$**	**$[RuL^1(H_2O)(AcO)]$**	**$[RuL^1(AcO)(PPh_3)]$**
C1	0.177	0.411	0.385	0.410	0.402
C2	0.269	0.137	0.185	0.170	0.181
C7	-0.087	-0.166	-0.163	-0.128	-0.175
$N1_{imine}$	-0.347	-0.314	-0.315	-0.340	-0.304
C8	-0.359	-0.300	-0.361	-0.307	-0.374
C9	-0.355	-0.348	-0.367	-0.349	-0.345
$N2_{imine}$	-0.209	-0.293	-0.308	-0.331	-0.275

C10	-0.165	-0.163	-0.190	-0.141	-0.179
C11	0.160	0.127	0.166	0.166	0.185
C12	0.344	0.395	0.329	0.402	0.379
(O)1	-0.538	-0.635	-0.539	-0.584	-0.537
(O)2	-0.523	-0.636	-0.593	-0.583	-0.543
H_2O	-	-0.899	-0.842	-0.900	-
P1	-	0.491	0.625	-	0.588
Ru	-	0.762	0.853	1.130	0.921
AcO	-	-	-	-0.394	-0.477
		Solvent methanol			
C1	0.157	0.361	0.388	0.390	0.384
C2	0.257	0.143	0.162	0.126	0.156
C7	-0.099	-0.196	-0.162	-0.137	-0.181
$N1_{imine}$	-0.357	-0.300	-0.313	-0.331	-0.306
C8	-0.358	-0.362	-0.361	-0.328	-0.371
C9	-0.362	-0.360	-0.368	-0.331	-0.363
$N2_{imine}$	-0.231	-0.288	-0.306	-0.317	-0.281
C10	-0.178	-0.216	-0.187	-0.140	-0.195
C11	0.145	0.128	0.158	0.127	0.165
C12	0.325	0.331	0.353	0.398	0.368
(O)1	-0.554	-0.577	-0.558	-0.623	-0.554
(O)2	-0.556	-0.614	-0.594	-0.592	-0.569
H_2O	-	-0.850	-0.860	-0.854	-
P1	-	0.592	0.632	-	0.594
Ru	-	0.649	0.867	1.267	0.897
AcO	-		-	-0.545	

Table S7. Condensed–to-atom Fukui Indexes for ligand (L^1) at gaseous state. (a) B3LYP/DGDZVP and (b) B3LYP/6-31G** basis sets.

(a) B3LYP/DGDZVP						
	Hirshfeld charge			**Fukui**		
Atom	N	N+1	N-1	f^-	f^+	f^0
C1	0.200	0.192	0.153	0.047	-0.008	0.173
C2	0.269	0.296	0.242	0.028	0.026	0.269
C3	-0.346	-0.303	-0.361	0.015	0.043	-0.332
C4	-0.224	-0.184	-0.238	0.014	0.040	-0.211
C5	-0.269	-0.215	-0.274	0.005	0.055	-0.244
C6	-0.329	-0.277	-0.324	-0.005	0.052	-0.301
C7	-0.108	-0.074	-0.155	0.047	0.034	-0.114
$N1_{imine}$	-0.328	-0.344	-0.383	0.055	-0.016	-0.364
C8	-0.371	-0.340	-0.309	-0.062	0.031	-0.324
C9	-0.365	-0.335	-0.300	-0.065	0.030	-0.318
$N2_{imine}$	-0.222	-0.198	-0.260	0.037	0.025	-0.229
C10	-0.168	-0.158	-0.229	0.061	0.010	-0.194
C11	0.166	0.169	0.135	0.032	0.003	0.152
C12	0.353	0.358	0.305	0.048	0.005	0.332
C13	-0.409	-0.373	-0.419	0.010	0.036	-0.396
C14	-0.226	-0.186	-0.257	0.031	0.039	-0.222
C15	-0.258	-0.222	-0.251	-0.007	0.036	-0.237
C16	-0.319	-0.283	-0.340	0.022	0.036	-0.312
(O)1	-0.539	-0.473	-0.588	0.048	0.066	-0.531
(O)2	-0.535	-0.527	-0.573	0.038	0.008	-0.550

(b) B3LYP/6-31G**						
	NPA charge			**Fukui**		
Atom	N	N+1	N-1	f^-	f^+	f^0
C1	-0.199	-0.139	-0.191	-0.008	0.059	-0.165
C2	0.387	0.444	0.360	0.027	0.057	0.402
C3	-0.297	-0.245	-0.319	0.021	0.053	-0.282
C4	-0.206	-0.200	-0.275	0.069	0.006	-0.237
C5	-0.282	-0.161	-0.289	0.007	0.121	-0.225
C6	-0.191	-0.195	-0.233	0.042	-0.004	-0.214
C7	0.122	0.117	0.033	0.088	-0.005	0.075
$N1_{imine}$	-0.528	-0.481	-0.589	0.061	0.047	-0.535
C8	-0.276	-0.282	-0.264	-0.012	-0.006	-0.273
C9	-0.285	-0.291	-0.274	-0.011	-0.006	-0.282
$N2_{imine}$	-0.461	-0.428	-0.525	0.064	0.033	-0.477
C10	0.091	0.089	0.021	0.070	-0.002	0.055

C11	-0.158	-0.116	-0.169	0.011	0.042	-0.143
C12	0.356	0.402	0.338	0.018	0.046	0.370
C13	-0.321	-0.314	-0.347	0.027	0.007	-0.331
C14	-0.209	-0.171	-0.286	0.077	0.038	-0.228
C15	-0.269	-0.211	-0.272	0.003	0.058	-0.241
C16	-0.180	-0.189	-0.231	0.051	-0.009	-0.210
(O)1	-0.703	-0.600	-0.732	0.030	0.103	-0.666
(O)2	-0.698	-0.651	-0.706	0.009	0.047	-0.679

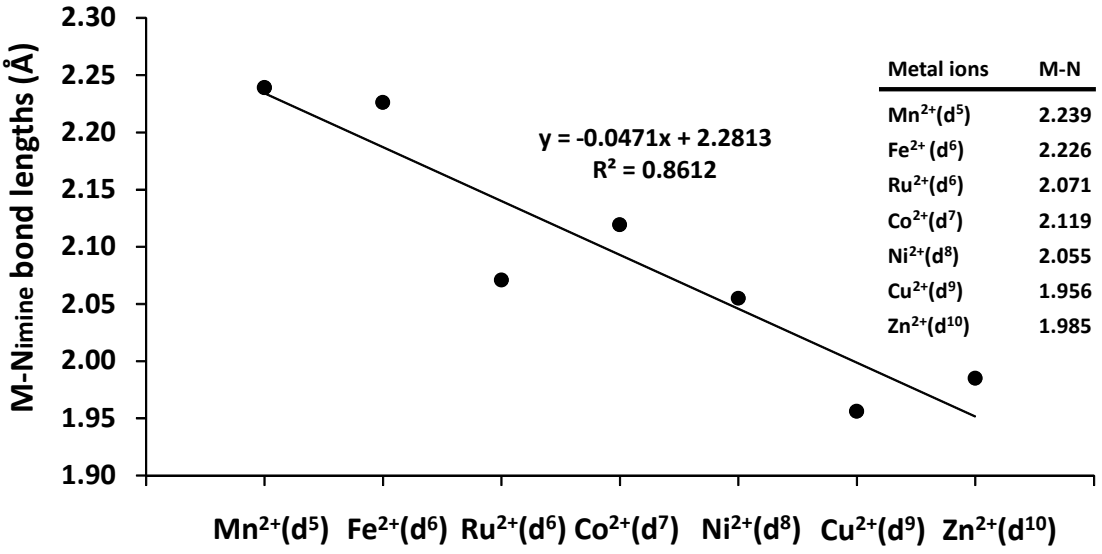


Fig. S1. The variation of bond length (M-Nimine) against the electron increase in the d-orbital of different divalent metal ions.

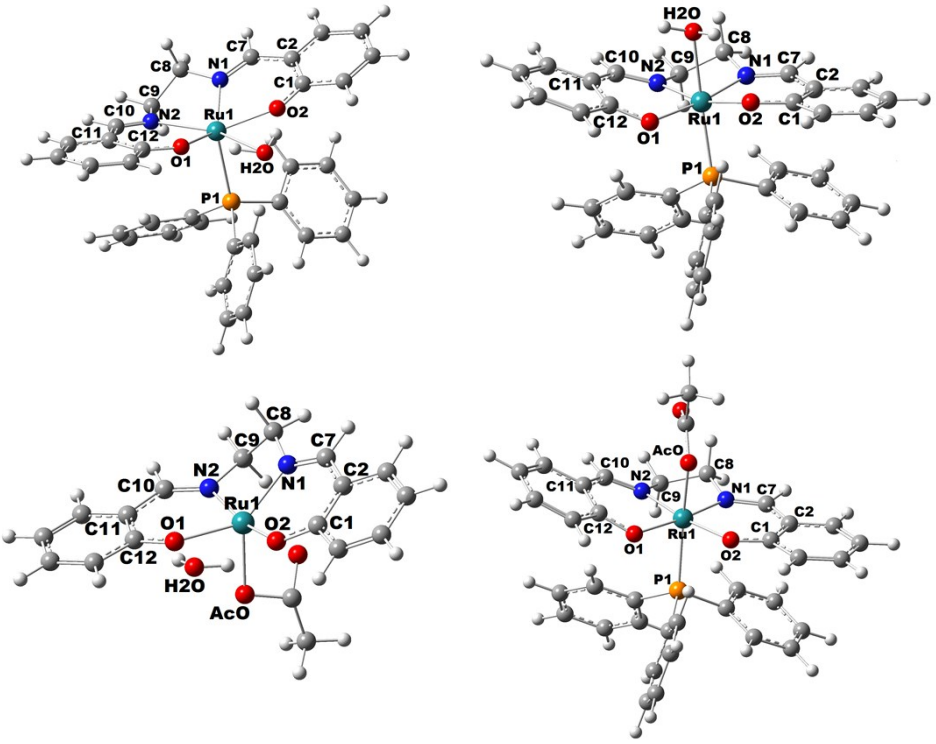


Fig. S2a. The optimized geometrical structural of $[RuL^1(H_2O)(PPh_3)]$, $[RuL^1(H_2O)(PPh_3)]^+$, $[RuL^1(H_2O)(AcO)]$ and $[RuL^1(AcO)(PPh_3)]$ at gaseous state

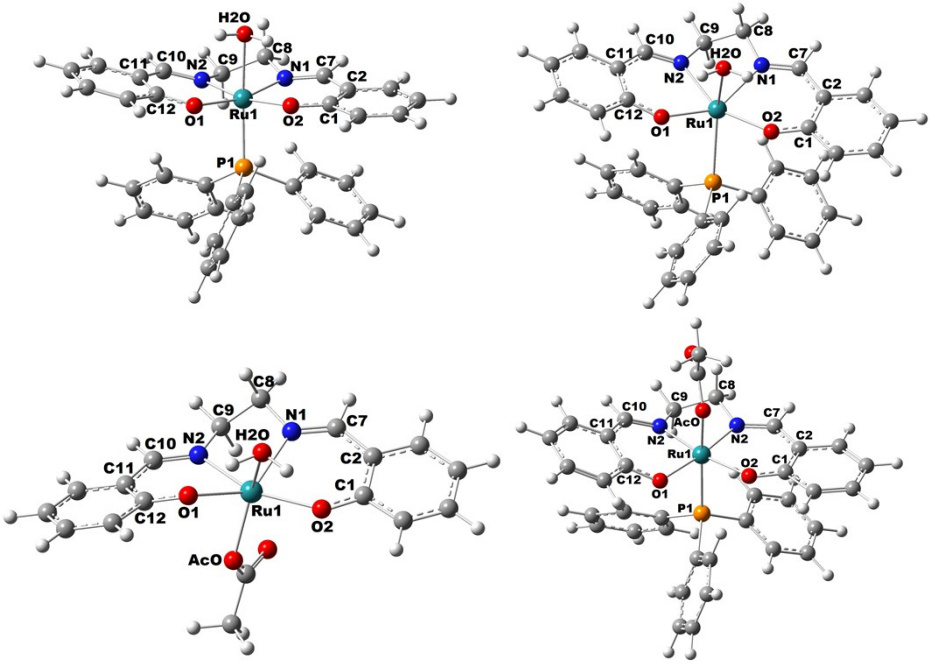
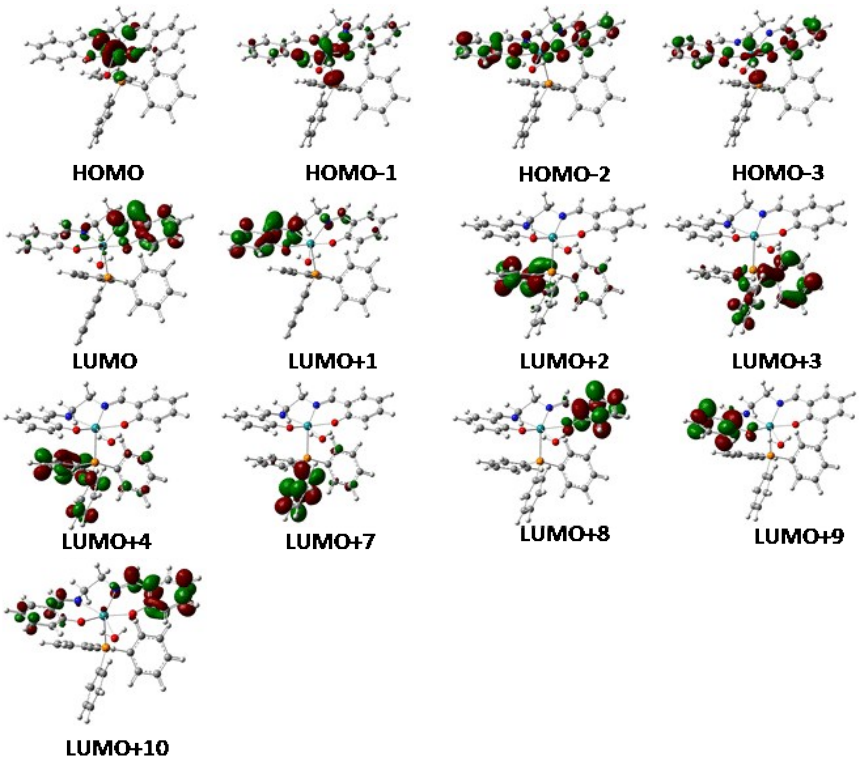


Fig. S2b. The optimized geometrical structural of $[RuL^1(H_2O)(PPh_3)]$, $[RuL^1(H_2O)(PPh_3)]^+$, $[RuL^1(H_2O)(AcO)]$ and $[RuL^1(AcO)(PPh_3)]$ in methanol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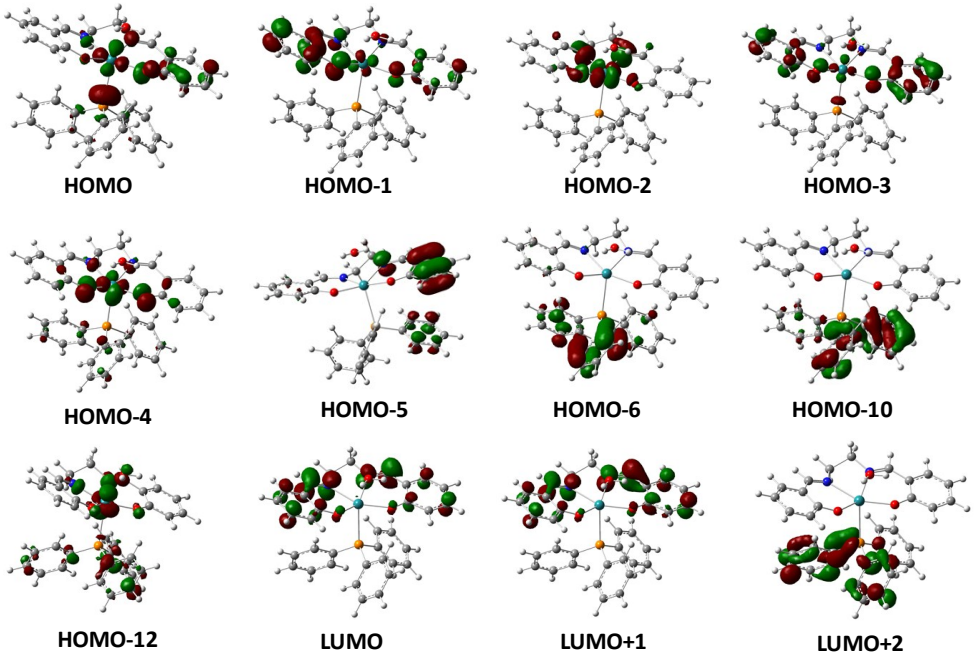
HOMO-2
HOMO-3
LUMO
LUMO+1
LUMO+2
LUMO+3
LUMO+4
LUMO+7
LUMO+8
LUMO+9
LUMO+10

a)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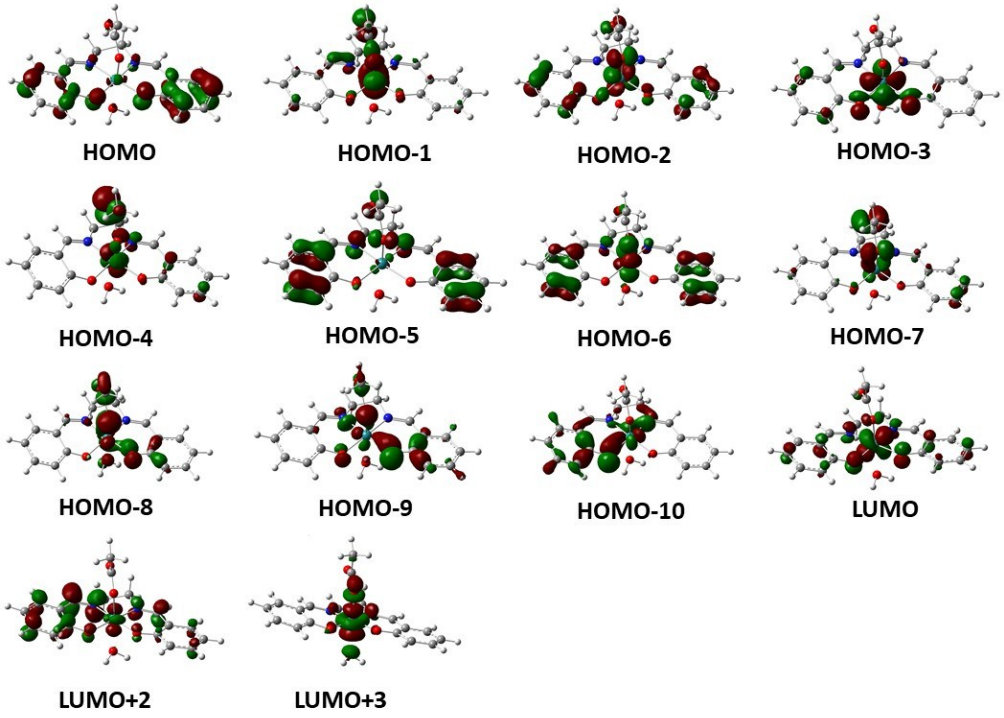
HOMO-2
HOMO-3
HOMO-4
HOMO-5
HOMO-6
HOMO-10
HOMO-12
LUMO
LUMO+1
LUMO+2

b)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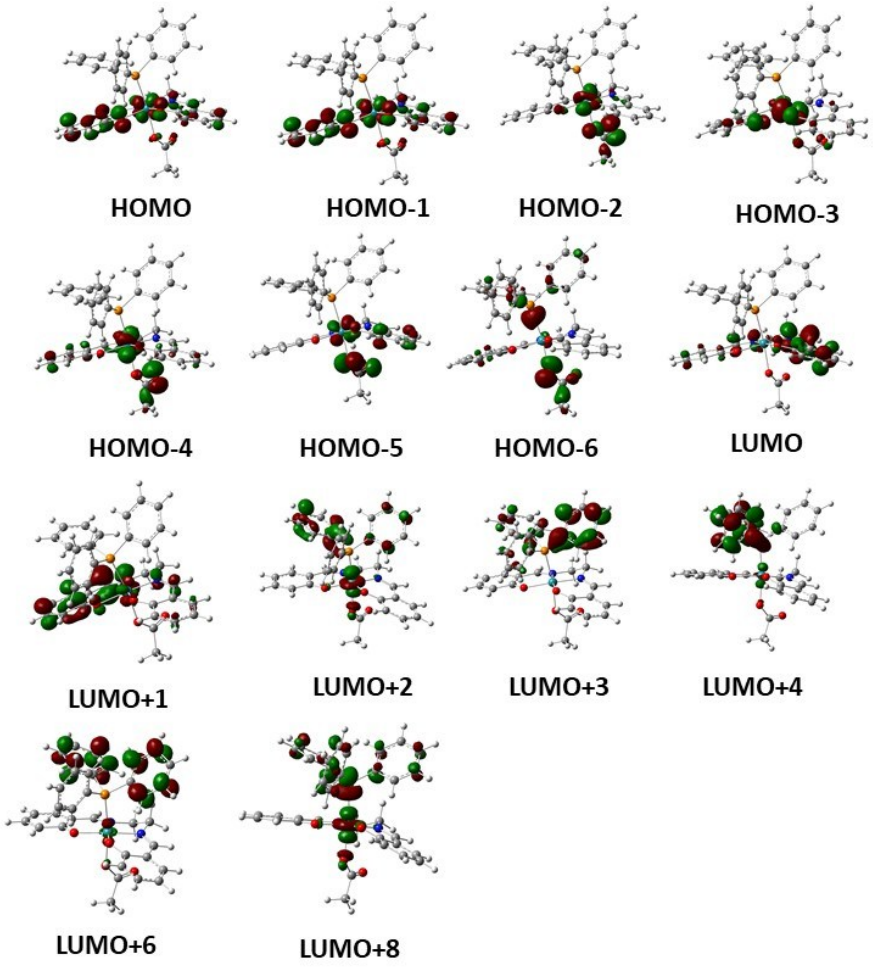
HOMO-1
HOMO-2
HOMO-3
HOMO-4
HOMO-5
HOMO-6
HOMO-7
HOMO-8
HOMO-9
HOMO-10
LUMO
LUMO+2
LUMO+3

c)



d)

Fig. S3. Frontier molecular orbitals (HOMOs and LUMOs) of complexes: a) $[RuL^1(H_2O)(PPh_3)]$, b) $[RuL^1(H_2O)(PPh_3)]^+$, c) $[RuL^1(H_2O)(AcO)]$ and d) $[RuL^1(AcO)(PPh_3)]$ at gaseous state.

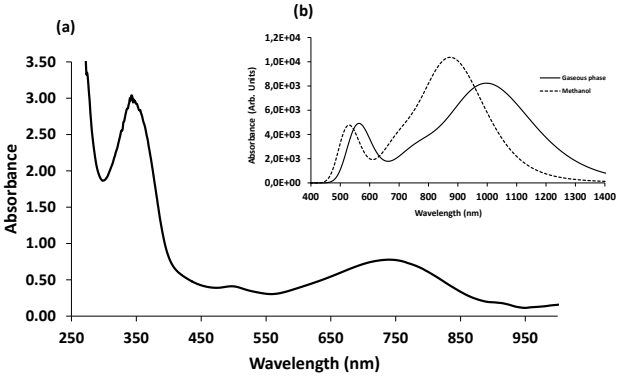


Fig. S4. a) Experimental UV-vis spectrum of $[RuL^1(H_2O)(PPh_3)]^+$; b) TD-DFT calculated spectrum using the B3LYP method in the gaseous state and considering methanol as solvent.

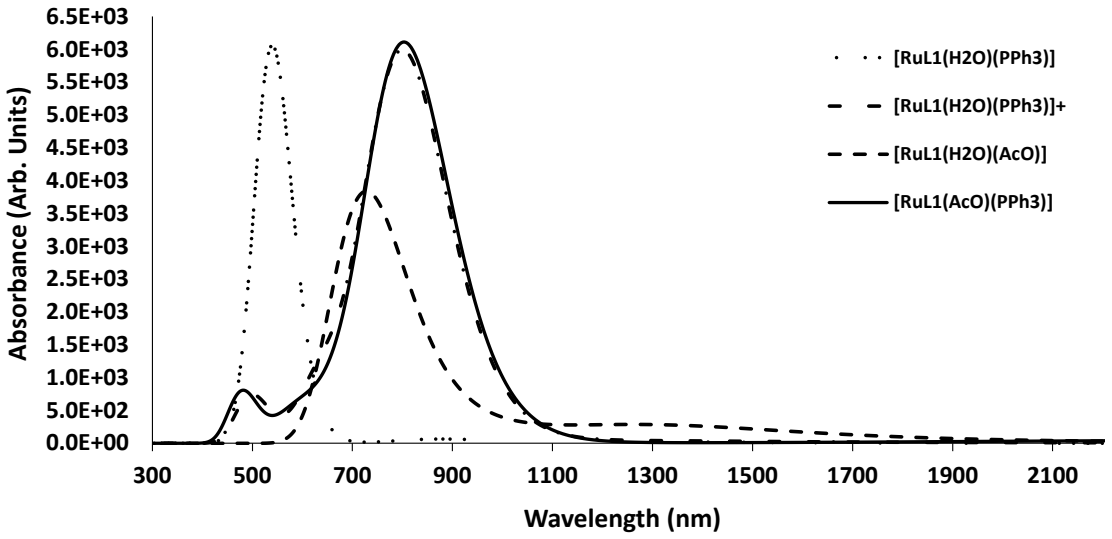


Fig. S5. TD-DFT spectra $[RuL^1(H_2O)(PPh_3)]$, $[RuL^1(H_2O)(PPh_3)]^+$ $[RuL^1(H_2O)(AcO)]$ and $[RuL^1(AcO)(PPh_3)]$ at gaseous state.

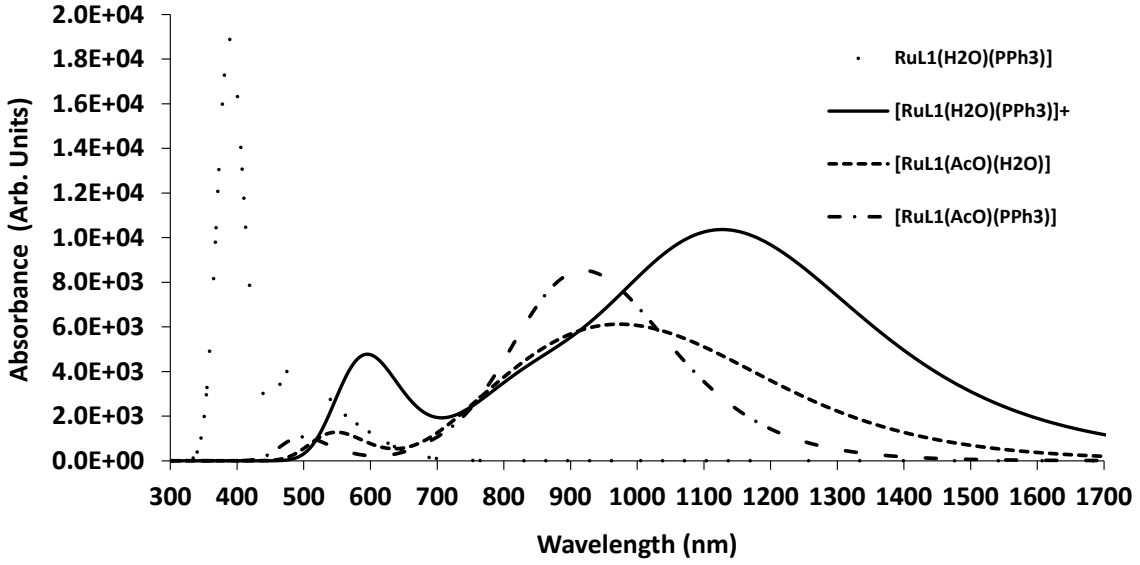


Fig. S6. TD-DFT spectra $[RuL^1(H_2O)(PPh_3)]$, $[RuL^1(H_2O)(PPh_3)]^+$ $[RuL^1(H_2O)(AcO)]$ and $[RuL^1(AcO)(PPh_3)]$ in methanol.

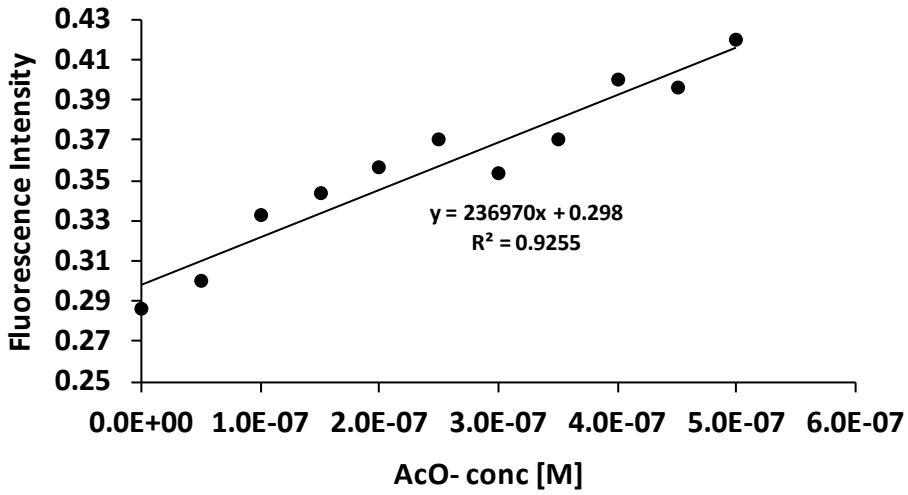
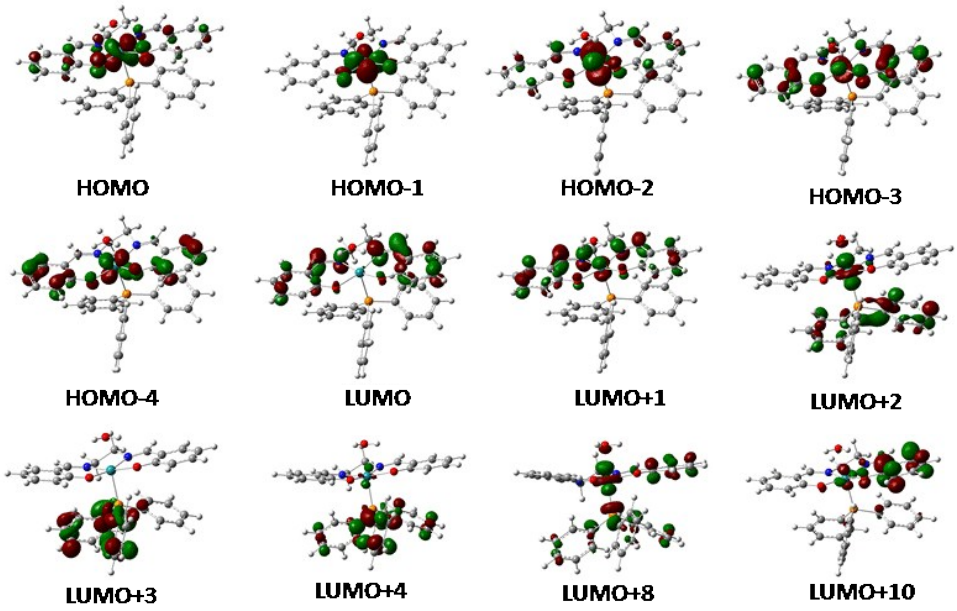
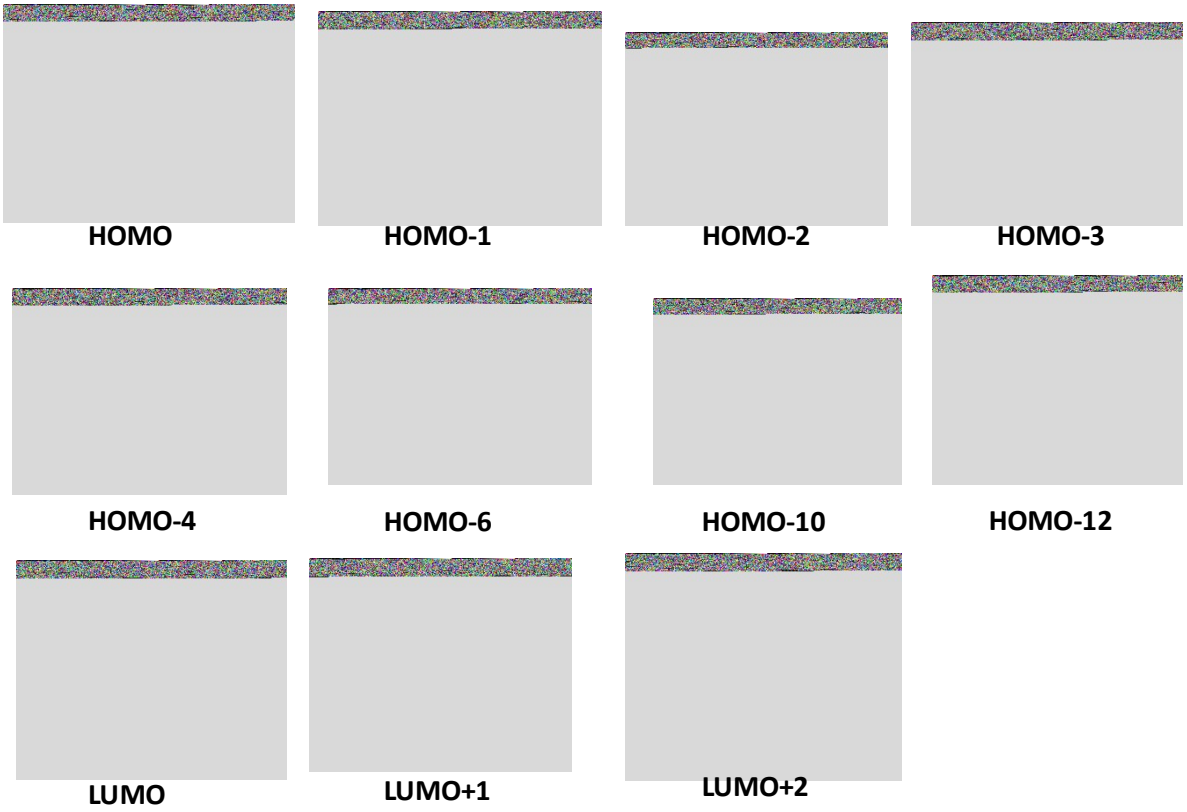


Fig. S7. Limited detection by Fluorescence titration of $[RuL^{1}(H_2O)(PPh^{3})]^{+}$ with AcO^{-} ions.



a)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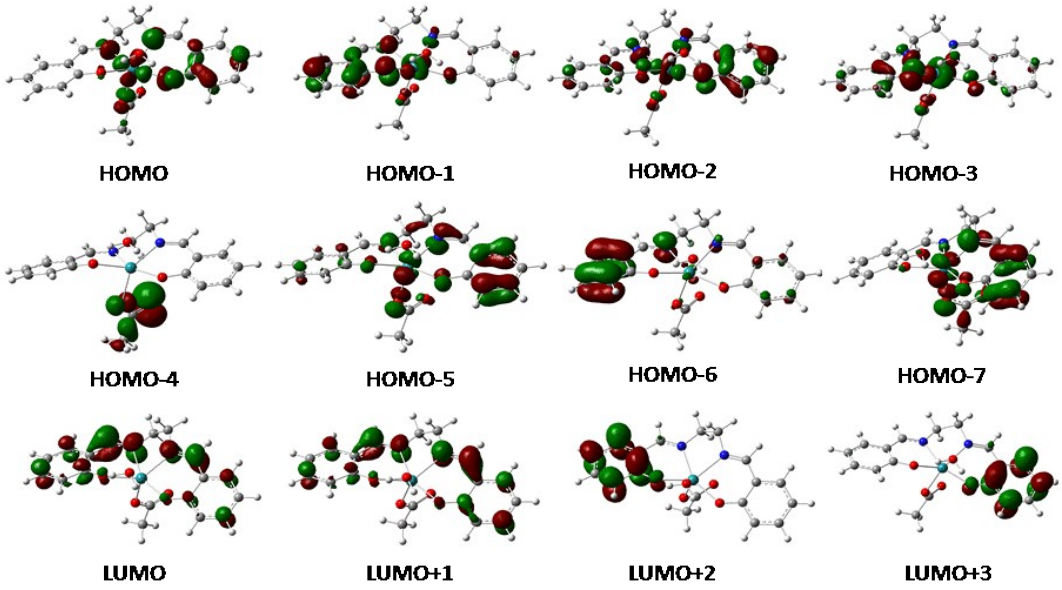
HOMO-1
HOMO-2
HOMO-3
HOMO-4
HOMO-6
HOMO-10
HOMO-12
LUMO
LUMO+1
LUMO+2

b)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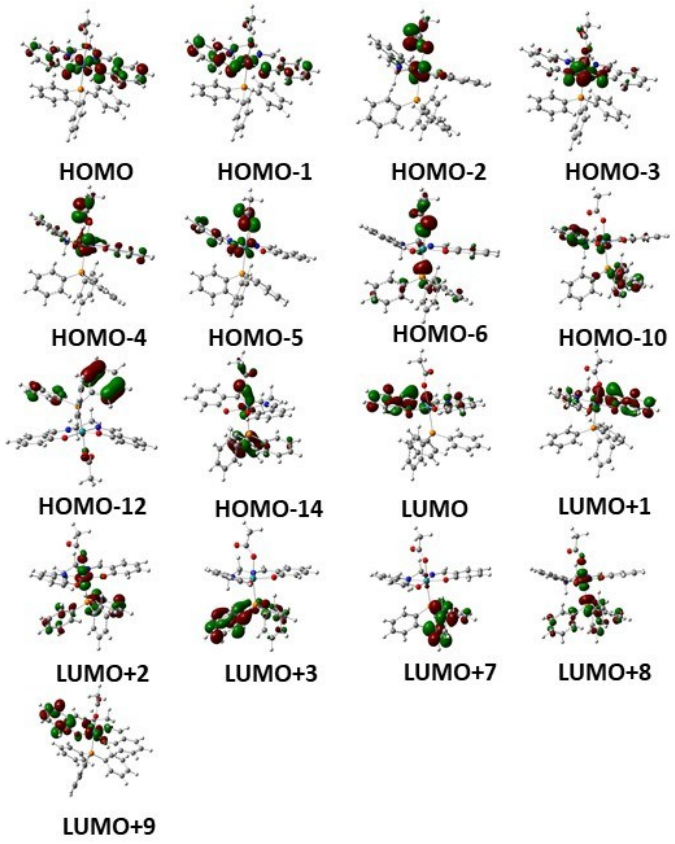
HOMO-1
HOMO-2
HOMO-3
HOMO-4
HOMO-5
HOMO-6
HOMO-7
LUMO
LUMO+1
LUMO+2
LUMO+3

c)



d)

Fig. S8. Frontier molecular orbitals (HOMOs and LUMOs) of complexes: a) $[RuL^1(H_2O)(PPh_3)]$, b) $[RuL^1(H_2O)(PPh_3)]^+$, c) $[RuL^1(H_2O)(AcO)]$ and d) $[RuL^1(AcO)(PPh_3)]$ in methanol.

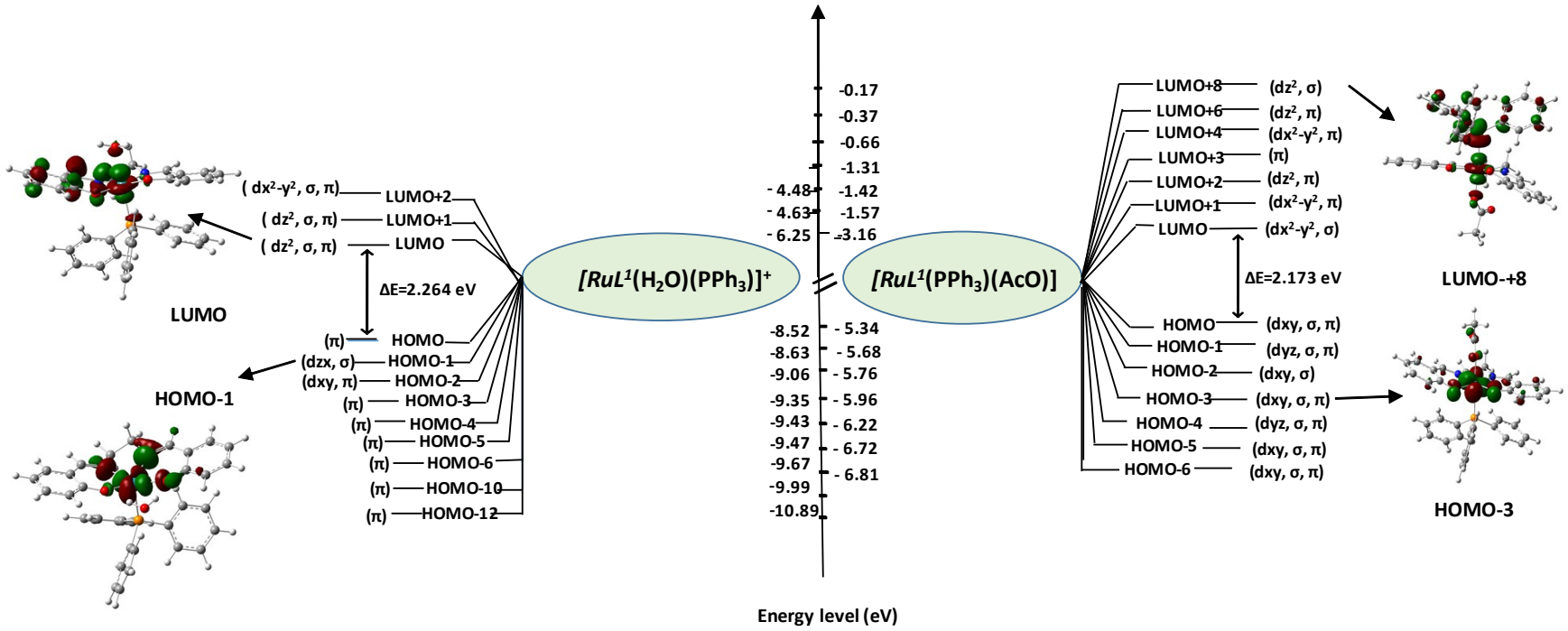


Fig. S9. Frontier molecular orbital energy level diagram of ruthenium complexes: a) $RuL^1(H_2O)(PPh_3)]^+$, b) $[RuL^1(AcO)(PPh_3)]$ and c)$[RuL^1(H_2O)(AcO)]$ at gaseous state.

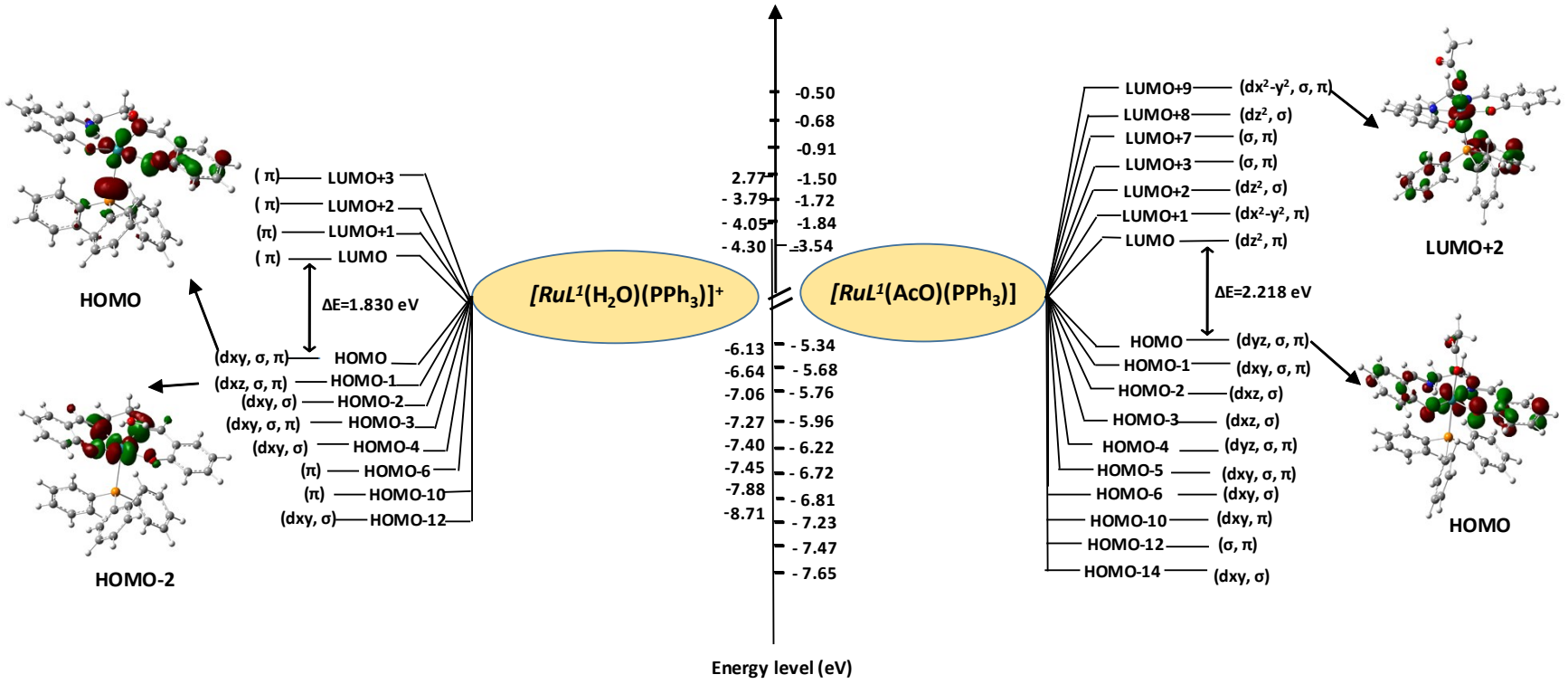


Fig. S10. Frontier molecular orbital energy level diagram of ruthenium complexes: a) $RuL^1(H_2O)(PPh_3)]^+$, b) $[RuL^1(AcO)(PPh_3)]$ and c)$[RuL^1(H_2O)(AcO)]$ in methanol (1/2).

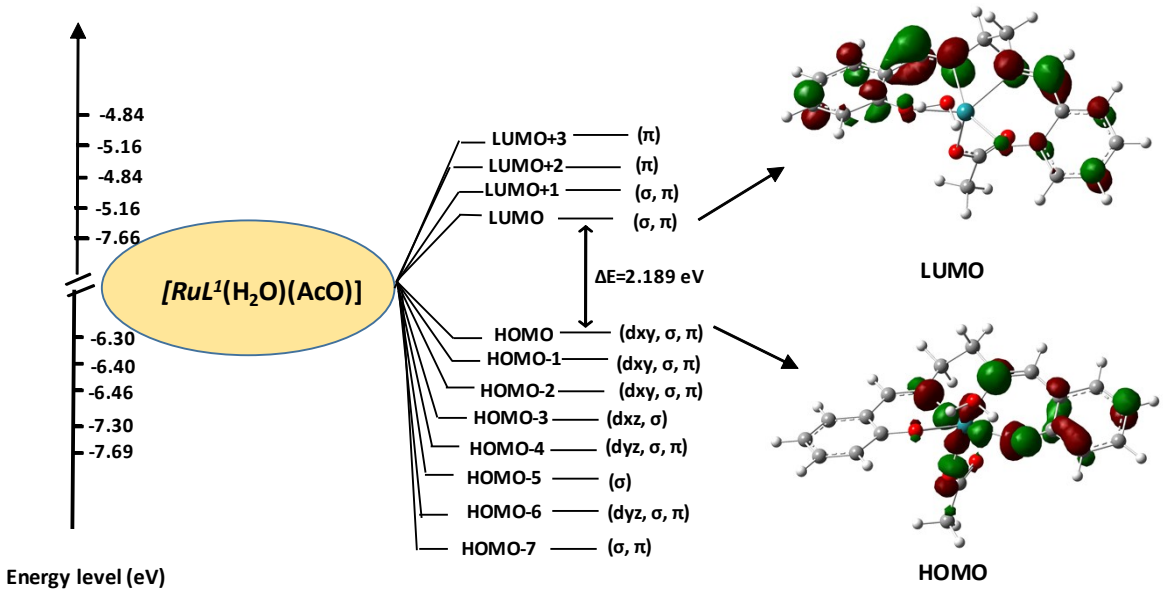


Fig. S11. Frontier molecular orbital energy level diagram of ruthenium complexes: a) $RuL^1(H_2O)(PPh_3)]^+$, b) $[RuL^1(AcO)(PPh_3)]$ and c)$[RuL^1(H_2O)(AcO)]$ in methanol (2/2).

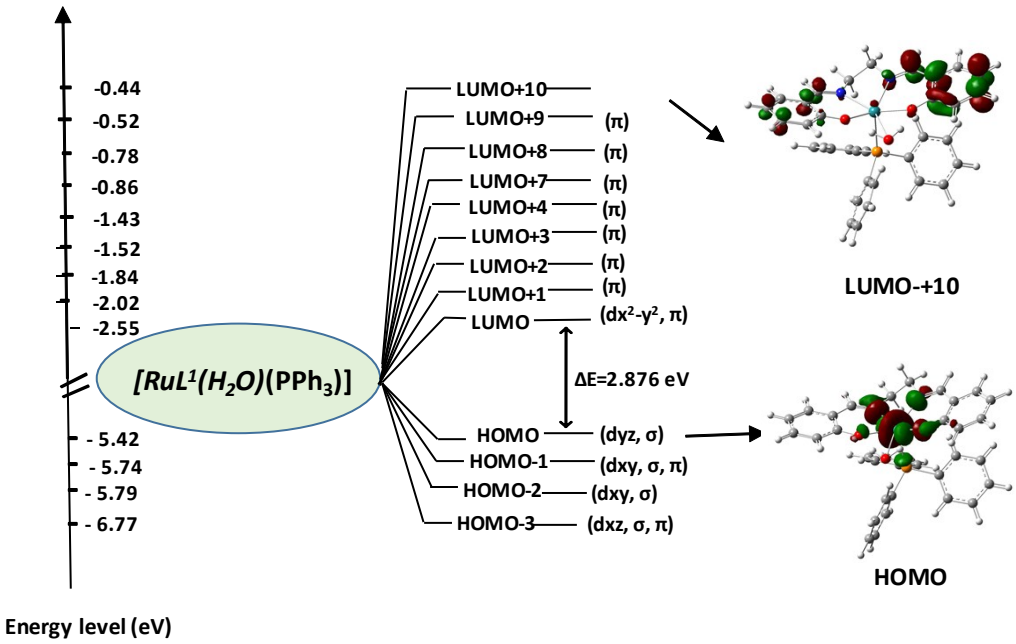


Fig S12. Frontier molecular orbital energy level diagram of ruthenium complexes: [Ru(L^1(H_2O(PPh_3)] at gaseous state.

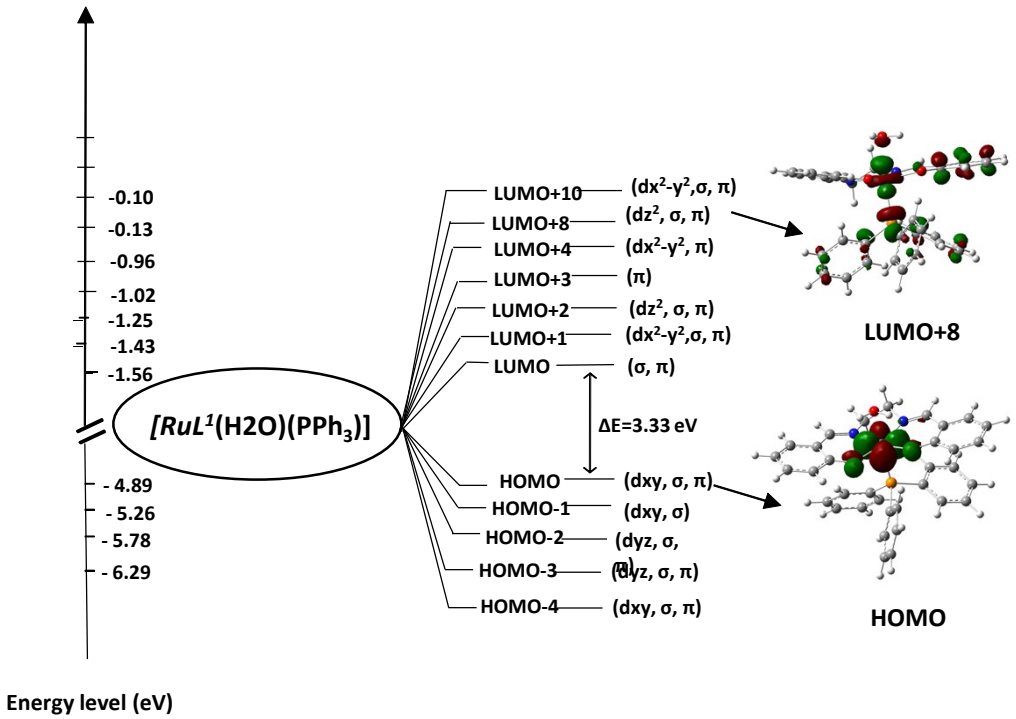
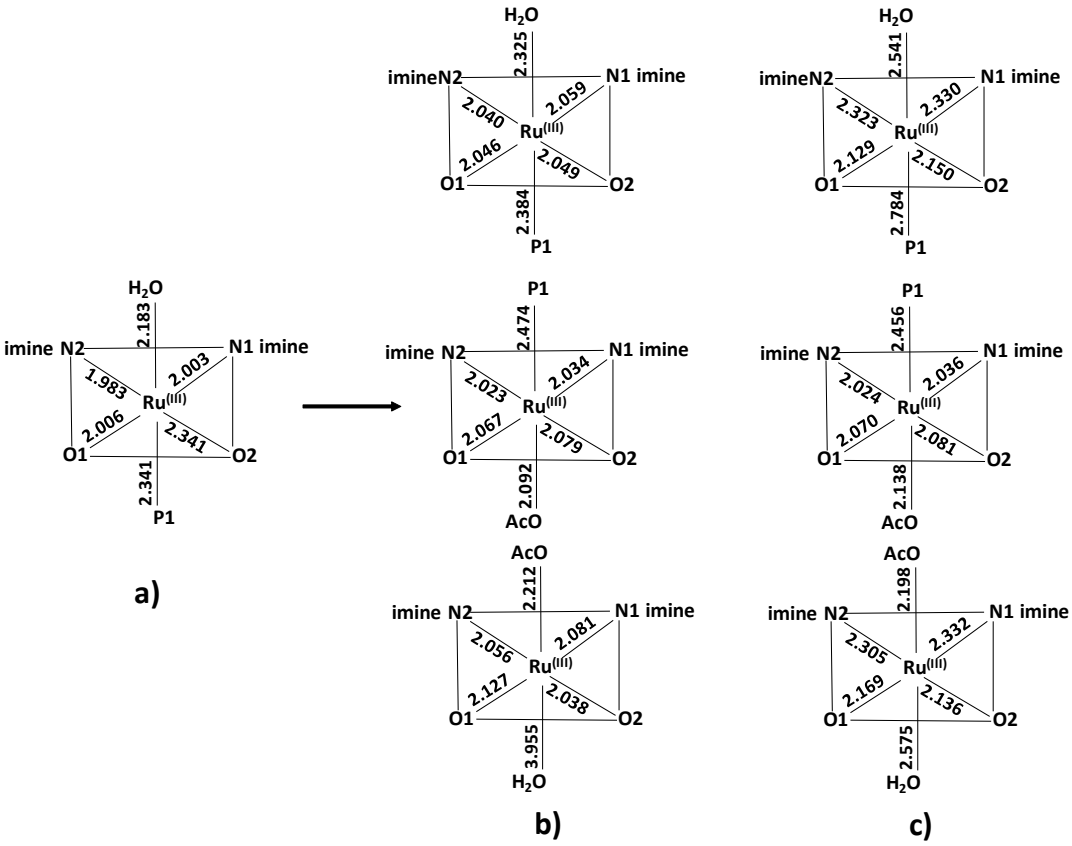
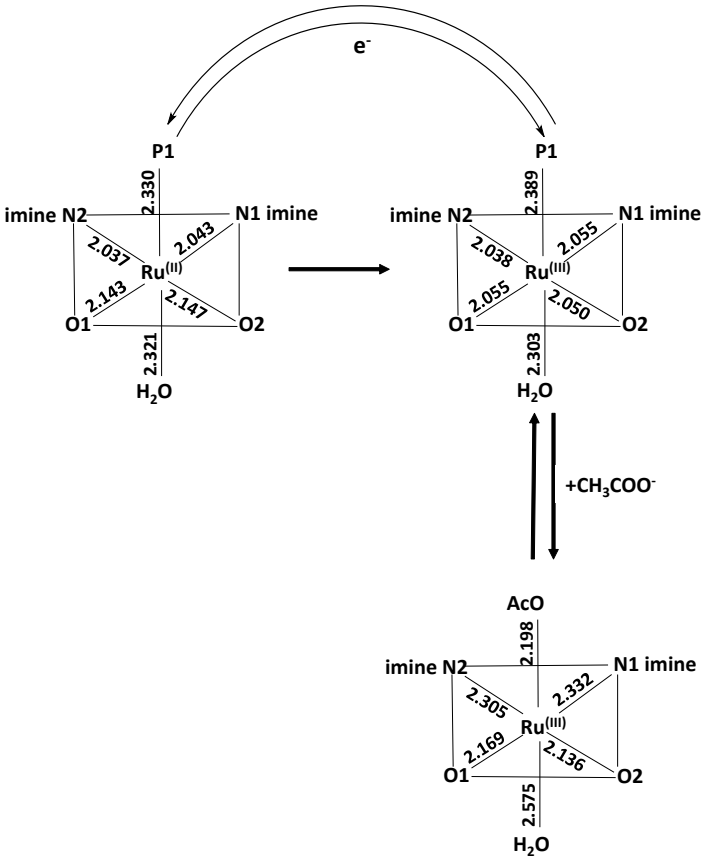


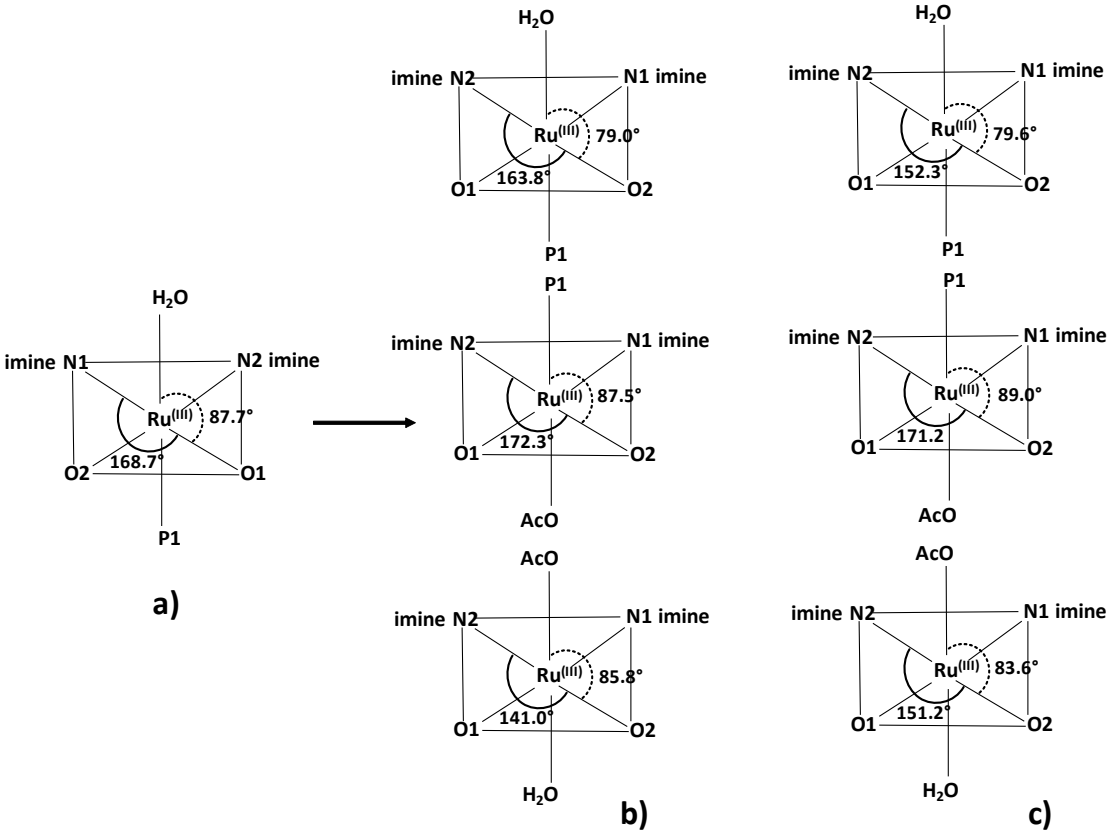
Fig S13. Frontier molecular orbital energy level diagram of ruthenium complexes: [Ru(L^1)(H_2O)(PPh_3)] in methanol.



Scheme S1. The variation of bond distances (axial and equatorial) during water and Phosphine substation in $[RuL^1(H_2O)(PPh_3)]^+$ by AcO^- ion. a) Experimental, b) gaseous state and c) methanol.



Scheme S2. The variation of bond distances (axial and equatorial) during oxidation in $[RuL^1(H_2O)(PPh_3)]$ to $[RuL^1(H_2O)(PPh_3)]^+$ in methanol



Scheme S3. The variation of Bond Angle (°) during water and Phosphine substation in $[RuL^1(H_2O)(PPh_3)]^+$ by AcO^- ion. a) Experimental, b) gaseous state and c) methanol.

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