Electronic Supplementary Information

Dual utility of a single diphosphine-ruthenium complex: a precursor for new complexes and, a pre-catalyst for transfer-hydrogenation and Oppenauer oxidation

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Table S1　　　Selected bond lengths (Å) and bond angles (°) for
[Ru(dppbz)(CO)(dmso)Cl$_2$]

| Bond lengths (Å)			
Ru1-Cl1	2.430(7)	C7-O1	1.09(2)
Ru1- Cl2	2.418(6)	P1-C1	1.843(18)
Ru1-P1	2.323(6)	C1-C6	1.35(2)
Ru1-P2	2.311(6)	P2-C2	1.811(17)
Ru1-C7	1.878(19)	S1-C8	1.85(2)
Ru1-S1	2.374(6)	S1-C9	1.74(2)
		S1-O2	1.465(16)
Bond angles (°)			
C7-Ru1-Cl2	176.9(7)	P1-Ru1-P2	82.75(17)
P1-Ru1-S1	178.1(2)	Ru1-C7-O1	177.6(18)
P2-Ru1-Cl1	173.21(17)		
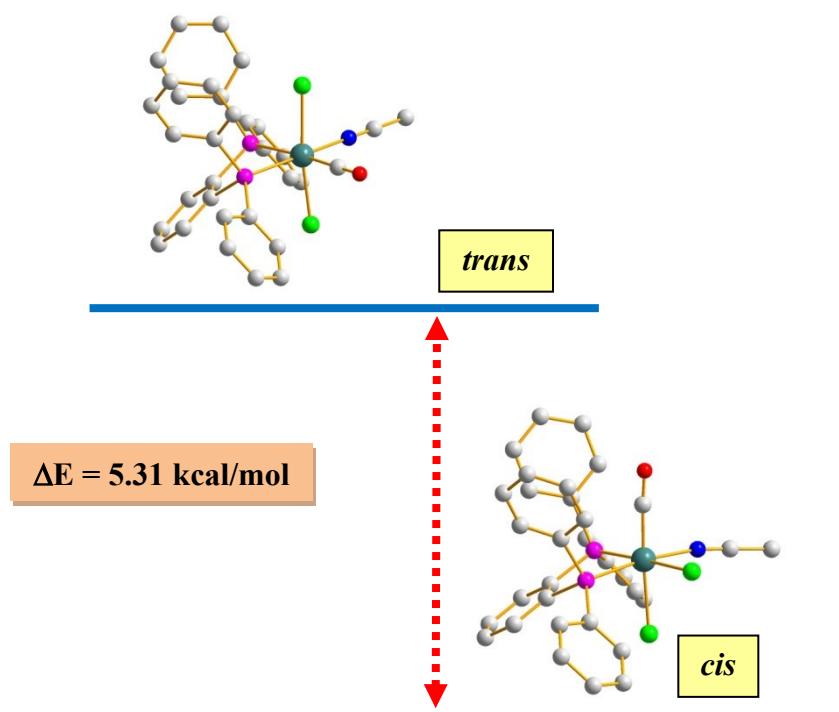
Fig. S1 DFT-optimized structures of the *cis* and *trans* isomers of the [Ru(dppbz)(CO)(CH$_3$CN)Cl$_2$], and the energy difference between them.
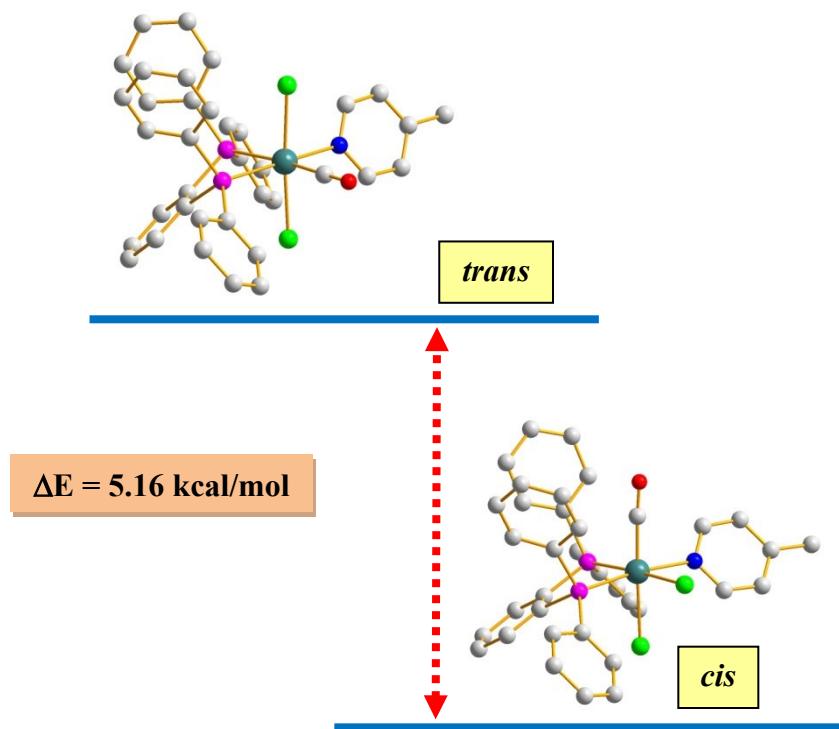
Fig. S2 DFT-optimized structures of the *cis* and *trans* isomers of the [Ru(dppbz)(CO)(4-picoline)Cl$_2$], and the energy difference between them.
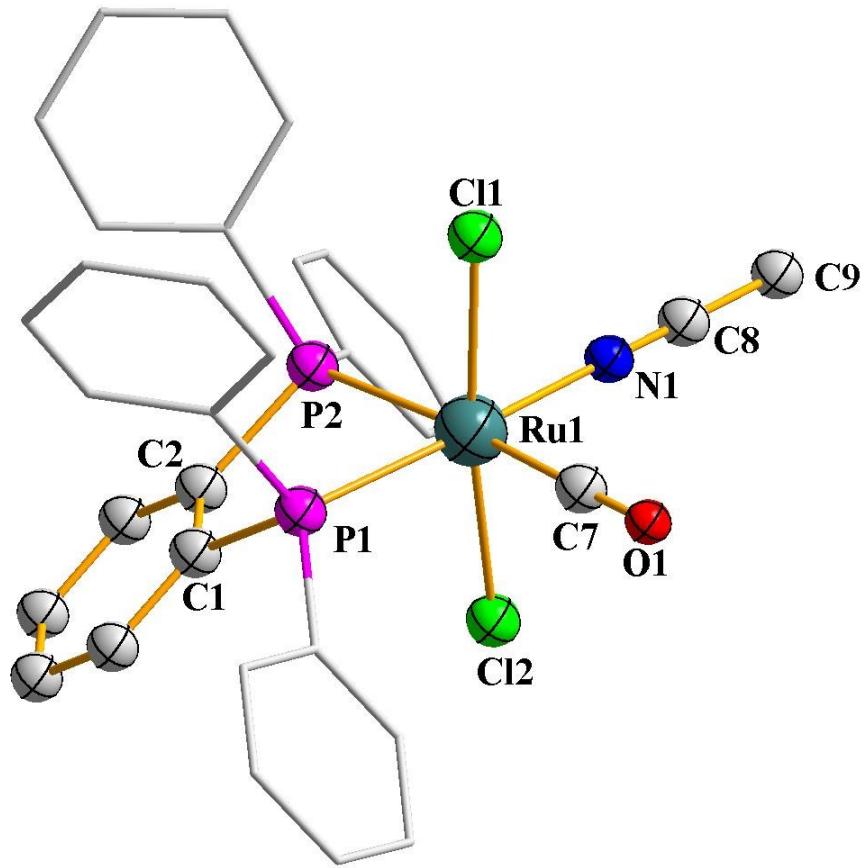
Fig. S3   DFT-optimized structure of [Ru(dppbz)(CO)(CH$_3$CN)Cl$_2$].
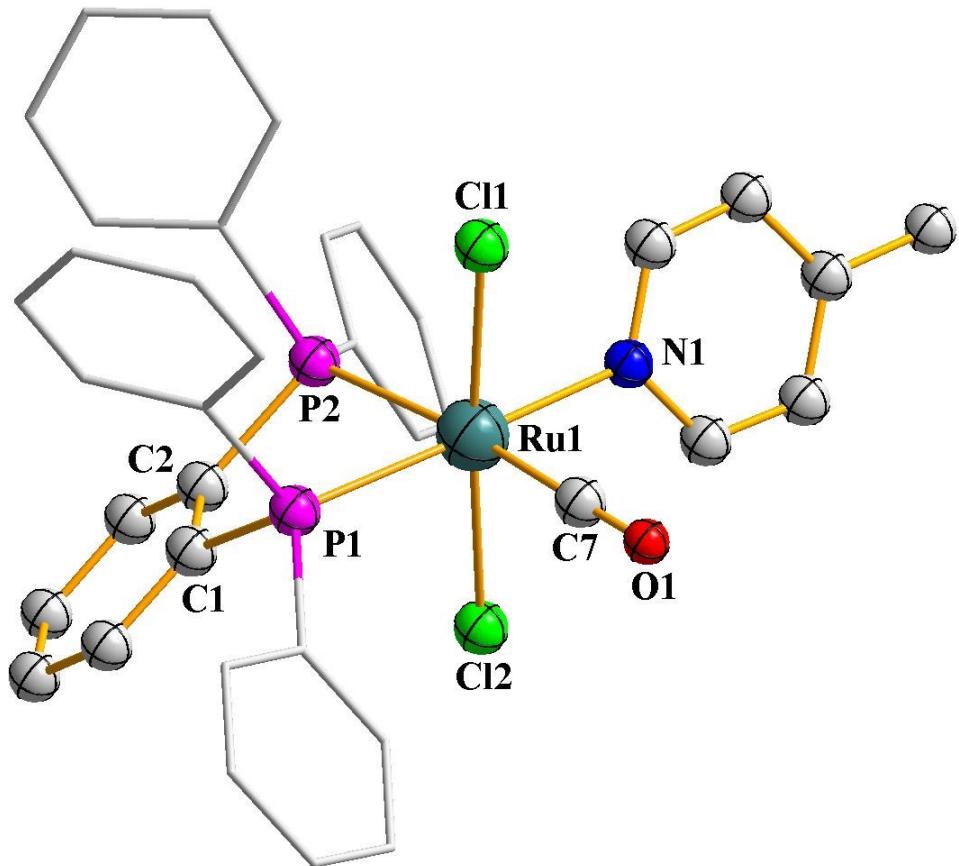
Fig. S4 DFT-optimized structure of [Ru(dppbz)(CO)(4-picoline)Cl$_2$].

Table S2   Selected bond lengths (Å) and bond angels (°) for the DFT-optimized structures of [Ru(dppbz)(CO)(CH$_3$CN)Cl$_2$] and [Ru(dppbz)(CO)(4-picoline)Cl$_2$] complexes.

[Ru(dppbz)(CO)(CH$_3$CN)Cl$_2$]		[Ru(dppbz)(CO)(4-picoline)Cl$_2$]	
Bond lengths (Å)			
Ru1-Cl1	2.475	Ru1-Cl1	2.482
Ru1-Cl2	2.506	Ru1-Cl2	2.512
Ru1-P1	2.362	Ru1-P1	2.367
Ru1-P2	2.494	Ru1-P2	2.523
Ru1-N1	2.103	Ru1-N1	2.237
Ru1-C7	1.904	Ru1-C7	1.892
C7-O1	1.152	C7-O1	1.153
C8-N1	1.155		
C8-C9	1.458		
Bond angles (°)			
Cl1-Ru1-Cl2	172.72	Cl1-Ru1-Cl2	175.61
P1-Ru1-N1	172.52	P1-Ru1-N1	173.23
P2-Ru1-C7	174.87	P2-Ru1-C7	174.31
P1-Ru1-P2	80.67	P1-Ru1-P2	79.75
Ru1-C7-O1	179.16	Ru1-C7-O1	179.22
Ru1-N1-C8	178.27		
N1-C8-C9	179.36		

Table S3　　Selected bond lengths (Å) and bond angles (°) for [Ru(dppbz)$_2$Cl$_2$].

Bond lengths (Å)			
Ru1-Cl1	2.4565(16)	P1-C1	1.821(3)
Ru1-P1	2.3944(6)	C1-C2	1.394(4)
Ru1-P2	2.4042(6)	C2-P2a	1.825(3)
Bond angles (°)			
Cl1-Ru1-Cl1a	180.00	P2-Ru1-P2a	180.00
P1-Ru1-P1a	180.00	P1-Ru1-P2	79.36(2)

Table S4   Selected bond lengths (Å) and bond angles (°) for [Ru(dppbz)(q)$_2$].

Bond lengths (Å)			
Ru1-P1	2.2499(13)	P1-C1	1.822(5)
Ru1-P2	2.2479(13)	C1-C2	1.384(6)
Ru1-O1	2.099(3)	C2-P2	1.842(5)
Ru1-O2	2.080(3)	C13-O1	1.319(6)
Ru1-N1	2.102(4)	C22-O2	1.327(7)
Ru1- N2	2.107(5)		
Bond angles (°)			
P1-Ru1-N1	179.34(10)	P1-Ru1-P2	83.95(5)
P2-Ru1-N2	172.27(13)	O1-Ru1-N1	79.52(13)
O1-Ru1-O2	167.65(13)	O2-Ru1-N2	79.87(16)

Table S5   Selected bond lengths (Å) and bond angles (°) for [Ru(dppbz)(pic)$_2$].

Bond lengths (Å)			
Ru1-P1	2.2505(14)	P1-C1	1.828(6)
Ru1-P2	2.2600(14)	C1-C2	1.386(8)
Ru1-O1	2.087(4)	C2-P2	1.829(6)
Ru1-O3	2.083(4)	C12-O1	1.290(8)
Ru1-N1	2.111(4)	C12-O2	1.237(9)
Ru1- N2	2.101(4)	C18-O3	1.294(9)
		C18-O4	1.253(8)
Bond angles (°)			
O1-Ru1-O3	167.32(14)	P1-Ru1-P2	83.83(5)
P1-Ru1-N1	171.21(16)	O1-Ru1-N1	79.35(19)
P2-Ru1-N2	176.19(13)	O3-Ru1-N2	78.77(17)

Table S6   Computed parameters from TDDFT calculations on
[Ru(dppbz)(CO)(dmso)Cl$_2$] for electronic spectral properties in
dichloromethane solution.

Excited state	Composition	CI value	E(eV)	Oscillator strength (*f*)	λ_{theo} (nm)	Assignment	λ_{exp} (nm)
1	H-18 → L	0.10734	3.7598	0.0217	329.76	ILCT/LLCT/MLCT /LMCT	340
	H-5 → L	0.15772				ILCT/MLCT /LMCT	
	H-3 → L	0.23743				LLCT/LMCT	
	H-2 → L	0.49455				ILCT/LLCT/MLCT /LMCT	
	H → L	0.20547				LLCT/MLCT /LMCT	
	H → L+2	0.20566				LLCT/MLCT	
2	H-10 → L	0.11599	4.2144	0.0350	294.19	ILCT/LMCT	302
	H-4 → L	0.58068				ILCT/LLCT/MLCT /LMCT	
	H-3 → L	0.24127				LLCT/LMCT	
	H-2 → L	0.15822				ILCT/LLCT/MLCT /LMCT	
	H-2 → L+2	0.11493				ILCT/LLCT/MLCT	
	H → L	0.10291				LLCT/MLCT /LMCT	
3	H-7 → L	0.16237	4.6237	0.0279	268.15	ILCT/LMCT	270
	H-4 → L+1	0.13737				ILCT/LLCT/MLCT	
	H-4 → L+2	0.42329				ILCT/LLCT/MLCT	
	H-3 → L+2	0.30880				LLCT	
	H-2 → L+2	0.25224				ILCT/LLCT/MLCT	
	H → L+2	0.13803				LLCT/MLCT	
	H → L+3	0.15924				LLCT/MLCT/ LMCT	

Table S7 Compositions of the molecular orbitals of [Ru(dppbz)(CO)(dmso)Cl$_2$] associated with the electronic spectral transitions.

Molecular orbital	% Contribution of fragments				
	Ru	dppbz	CO	dmso	Cl
HOMO(H)	32	4	4	1	59
H-2	16	13	2	10	59
H-3	4	8	1	1	86
H-4	14	56	1	20	9
H-5	11	73	1	6	9
H-7	6	86	0	5	3
H-10	2	94	0	3	1
H-18	30	39	4	4	23
LUMO(L)	27	61	1	5	6
L+1	7	90	0	1	2
L+2	2	97	0	0	1
L+3	38	41	8	5	8

HOMO (H)	LUMO (L)
H-2	L+1
H-3	L+2
H-4	L+3
H-5	H-7
H-10	H-18
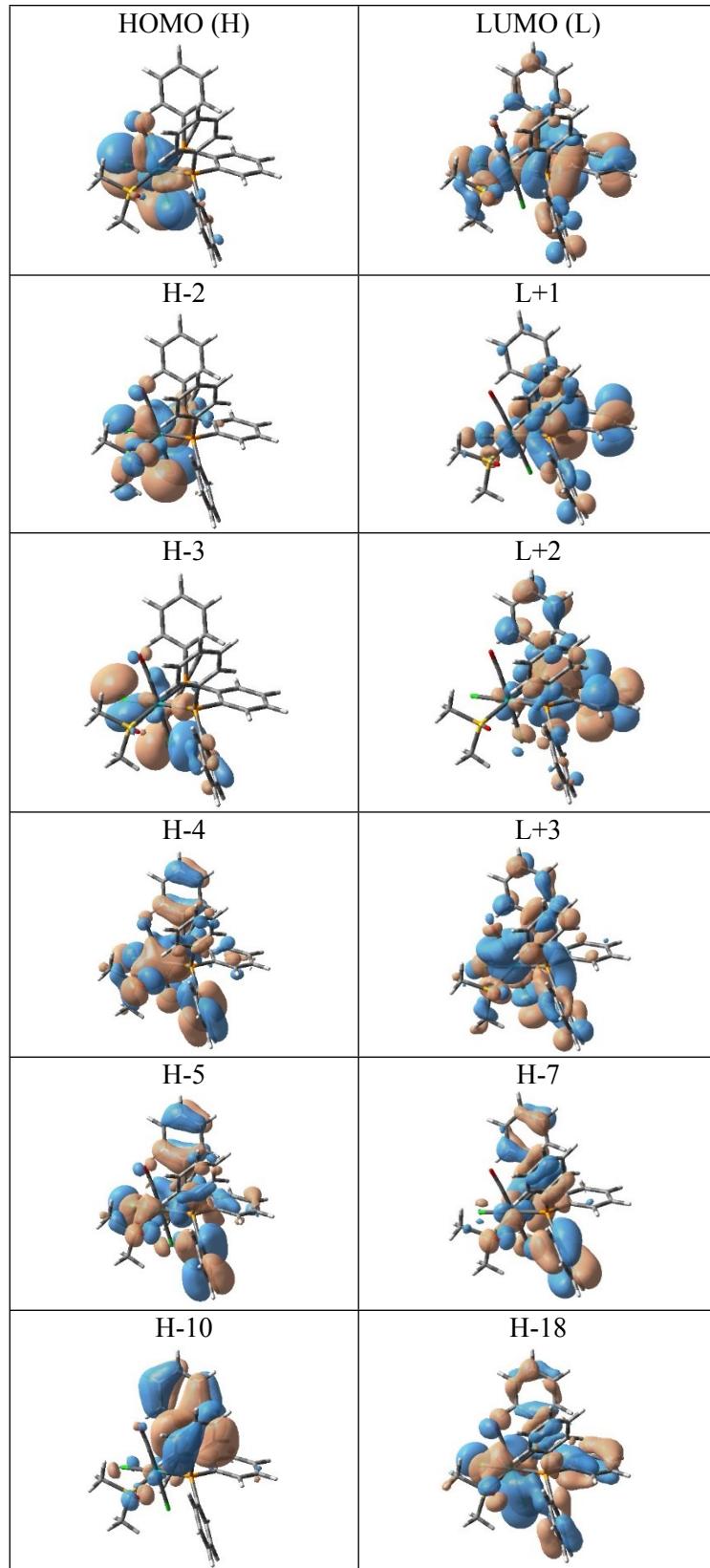
Fig. S5   Contour plots of selected molecular orbitals of [Ru(dppbz)(CO)(dmso)Cl$_2$].

Table S8 Computed parameters from TDDFT calculations on [Ru(dppbz)(CO)(CH$_3$CN)Cl$_2$] for electronic spectral properties in dichloromethane solution.

Excited state	Composition	CI value	E(eV)	Oscillator strength (f)	λ_{theo} (nm)	Assignment	λ_{exp} (nm)
1	H → L+1	0.49036	3.6494	0.0017	339.74	LLCT/ILCT/MLCT /LMCT	356
	H → L+2	0.32423				LLCT/MLCT	
	H → L+3	0.30759				LLCT/MLCT	
	H → L+13	0.11015				LLCT/MLCT	
2	H → L+1	0.11661	4.1561	0.0074	298.32	LLCT/ILCT/MLCT /LMCT	316
	H → L+2	0.35991				LLCT/MLCT	
	H → L+3	0.52997				LLCT/MLCT	
	H → L+6	0.11029				LLCT/MLCT	
	H → L+9	0.11197				LLCT/MLCT	
3	H-12 → L	0.10568	4.6578	0.0145	266.18	LLCT/ILCT	268
	H-8 → L	0.17308				LLCT/ILCT/MLCT	
	H-7 → L	0.18918				ILCT/MLCT	
	H-5 → L	0.38601				LLCT/ILCT	
	H-4 → L	0.37512				ILCT/MLCT	
	H-2 → L	0.19336				LLCT/ILCT	
	H → L+5	0.11095				LLCT/MLCT	

Table S9 Compositions of the molecular orbitals of [Ru(dppbz)(CO)(CH$_3$CN)Cl$_2$] associated with the electronic spectral transitions.

Molecular orbital	% Contribution of fragments				
	Ru	dppbz	CO	CH$_3$CN	Cl
HOMO(H)	47	3	0	2	48
H-2	8	25	4	1	62
H-4	14	78	2	2	4
H-5	8	80	1	1	10
H-7	19	73	2	2	4
H-8	23	62	2	2	11
H-12	3	84	0	1	12
LUMO(L)	5	92	1	1	1
L+1	43	33	1	3	20
L+2	8	87	3	1	1
L+3	9	87	2	1	1
L+5	2	96	1	1	0
L+6	4	92	2	1	1
L+9	8	65	16	11	0
L+13	2	12	4	82	0

HOMO (H)	LUMO (L)
H-2	L+1
H-4	L+2
H-5	L+3

H-7	L+5
H-8	L+6
H-12	L+9

L+13
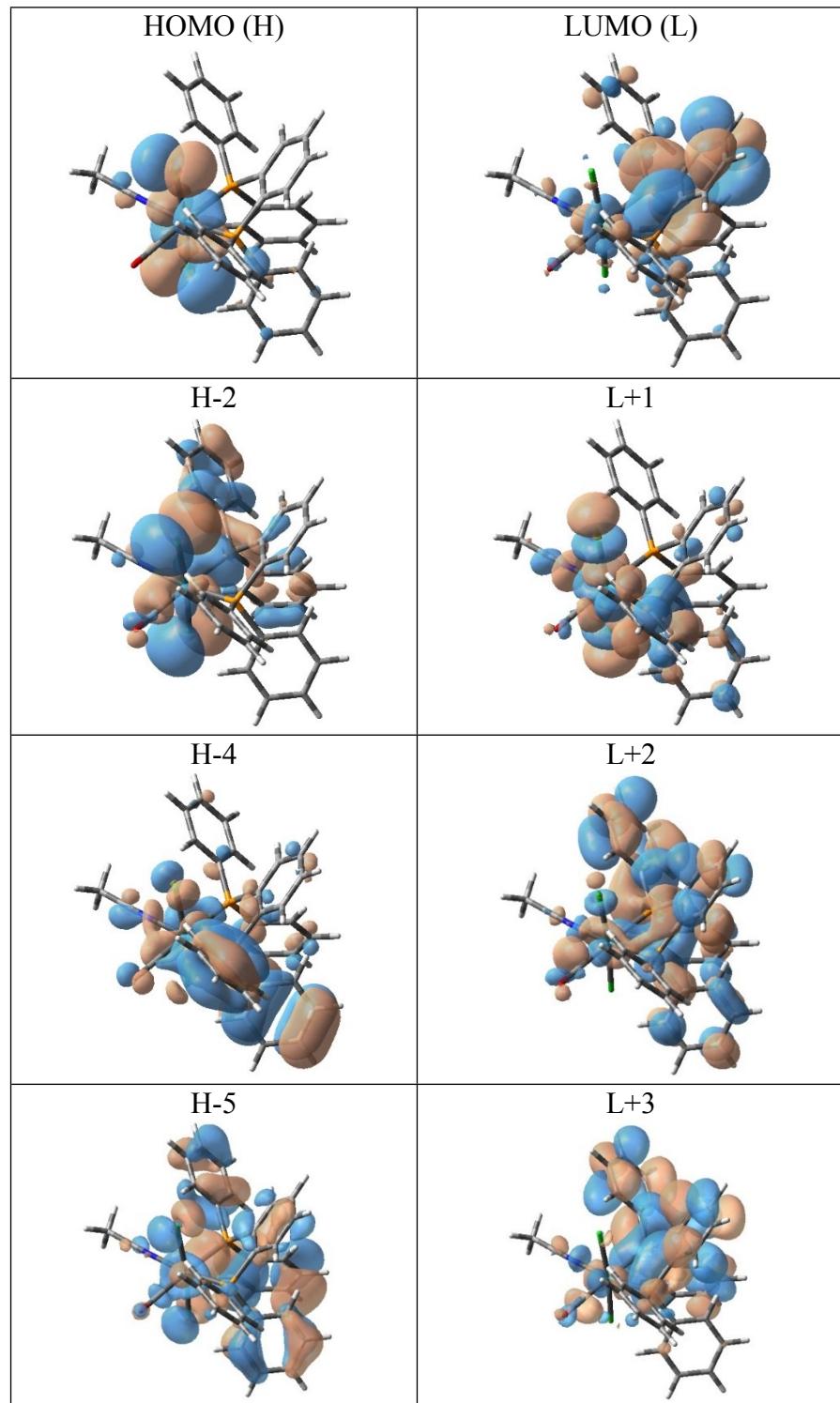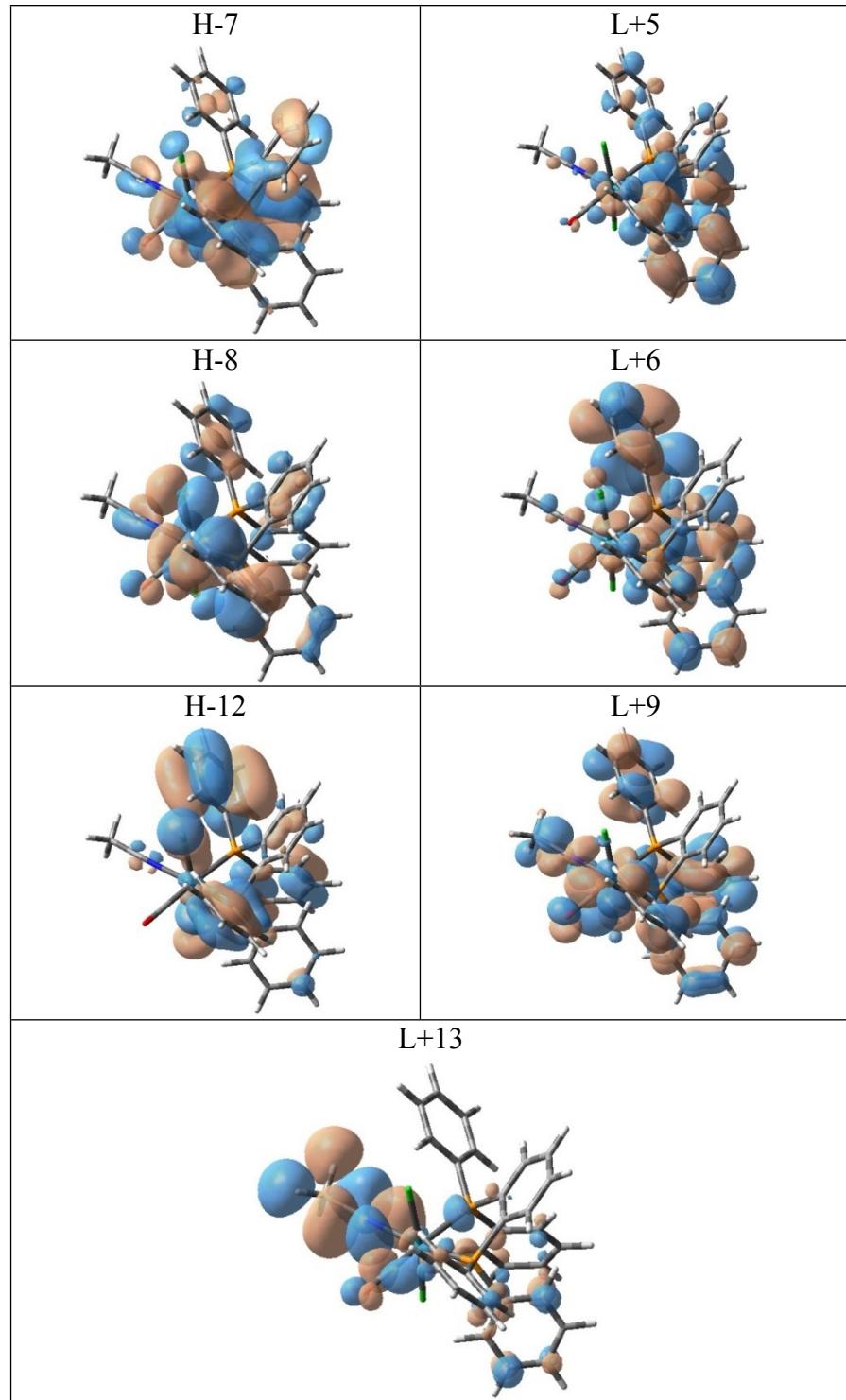
Fig. S6   Contour plots of selected molecular orbitals of [Ru(dppbz)(CO)(CH$_3$CN)Cl$_2$].

Table S10 Computed parameters from TDDFT calculations on [Ru(dppbz)(CO)(4-picoline)Cl$_2$] for electronic spectral properties in dichloromethane solution.

Excited state	Composition	CI value	E(eV)	Oscillator strength (f)	λ_{theo} (nm)	Assignment	λ_{exp} (nm)
1	H → L+1	0.57979	3.5210	0.0010	352.13	LLCT/MLCT /LMCT	363
	H → L+3	0.24482				LLCTMLCT	
	H → L+4	0.18434				LLCT/MLCT	
	H → L+5	0.10941				LLCT/MLCT	
	H → L+15	0.12413				LLCT/MLCT /LMCT	
2	H → L+1	0.17324	3.9611	0.0224	313.01	LLCT/MLCT /LMCT	307
	H → L+2	0.65465				LLCT/MLCT /LMCT	
3	H-11 → L	0.15677	4.7158	0.0529	262.91	LLCT/ILCT	269
	H-10 → L	0.11479				LLCT/ILCT	
	H-8 → L	0.19813				LLCT/ILCT	
	H-4 → L+1	0.10486				LLCT/ILCT/MLCT/ LMCT	
	H-3 → L	0.15915				LLCT/ILCT	
	H-2 → L+1	0.31018				LLCT/ILCT/MLCT/ LMCT	
	H-2 → L+3	0.10239				LLCT/ILCT/MLCT/ LMCT	
	H-1 → L+5	0.13393				LLCT/MLCT /LMCT	
	H-1 → L+6	0.28398				LLCT/MLCT	
	H-1 → L+7	0.13640				LLCT/MLCT	
	H-1 → L+9	0.10839				LLCT/MLCT	
	H-1 → L+12	0.13624				LLCT/MLCT	
	H → L+8	0.10219				LLCT/MLCT	

Table S11   Compositions of the molecular orbitals of [Ru(dppbz)(CO)(4-picoline)Cl$_2$] associated with the electronic spectral transitions.

Molecular orbital	% Contribution of fragments				
	Ru	dppbz	CO	4-picoline	Cl
HOMO(H)	54	3	0	2	41
H-1	43	3	3	0	51
H-2	18	37	5	3	37
H-3	10	30	1	3	56
H-4	23	63	2	6	6
H-8	1	86	0	1	12
H-10	8	82	0	1	9
H-11	4	79	0	1	16
LUMO(L)	8	55	1	36	0
L+1	21	29	1	41	8
L+2	23	49	1	18	9
L+3	12	70	5	9	4
L+4	5	86	2	7	0
L+5	12	80	4	1	3
L+6	2	62	1	35	0
L+7	1	52	0	47	0
L+8	4	94	1	0	1
L+9	6	90	1	2	1
L+12	4	83	12	1	0
L+15	20	41	38	1	0

HOMO (H)	LUMO (L)
H-1	L+1
H-2	L+2
H-3	L+3

H-4	L+4
H-8	L+5
H-10	L+6
H-11	L+7
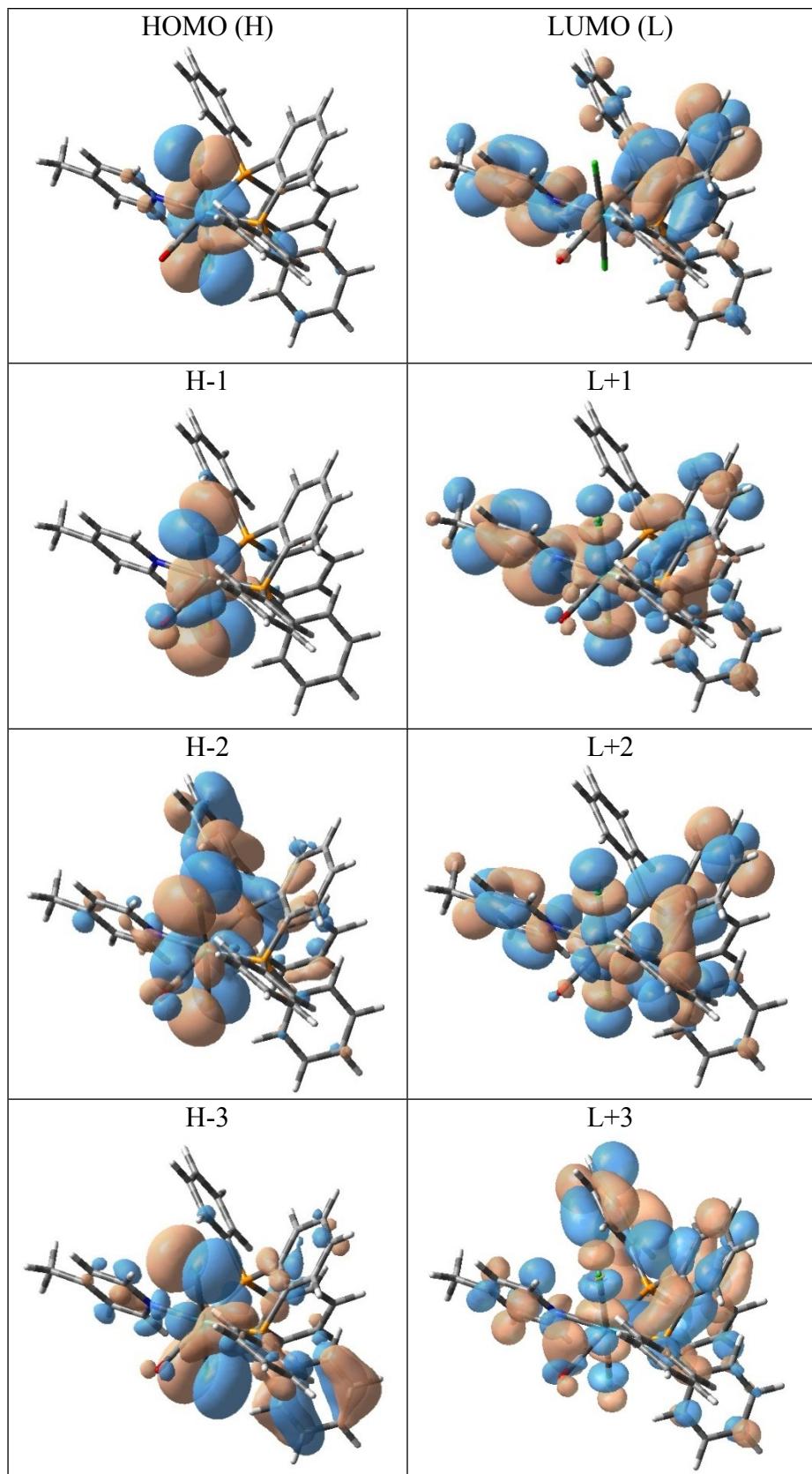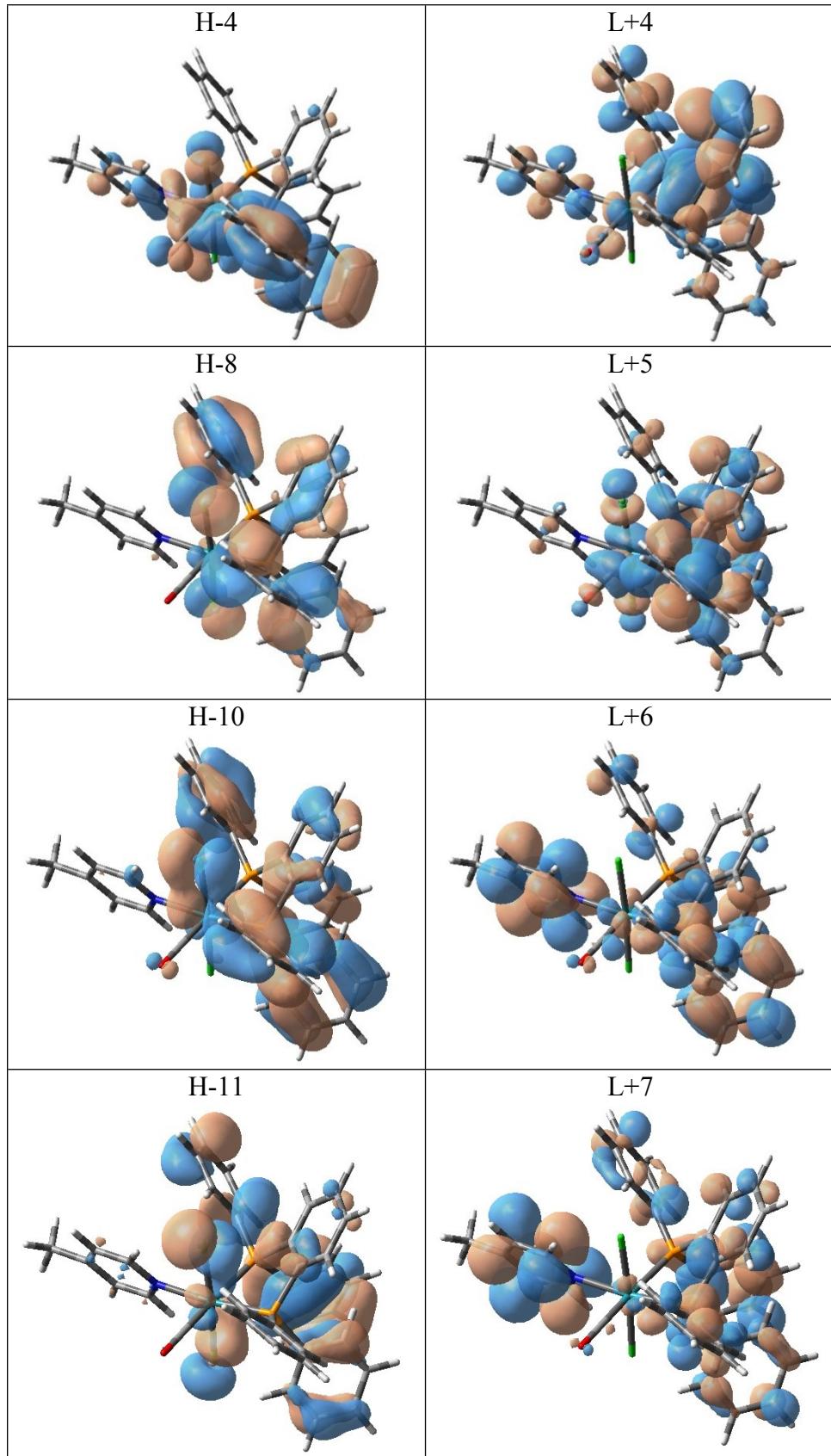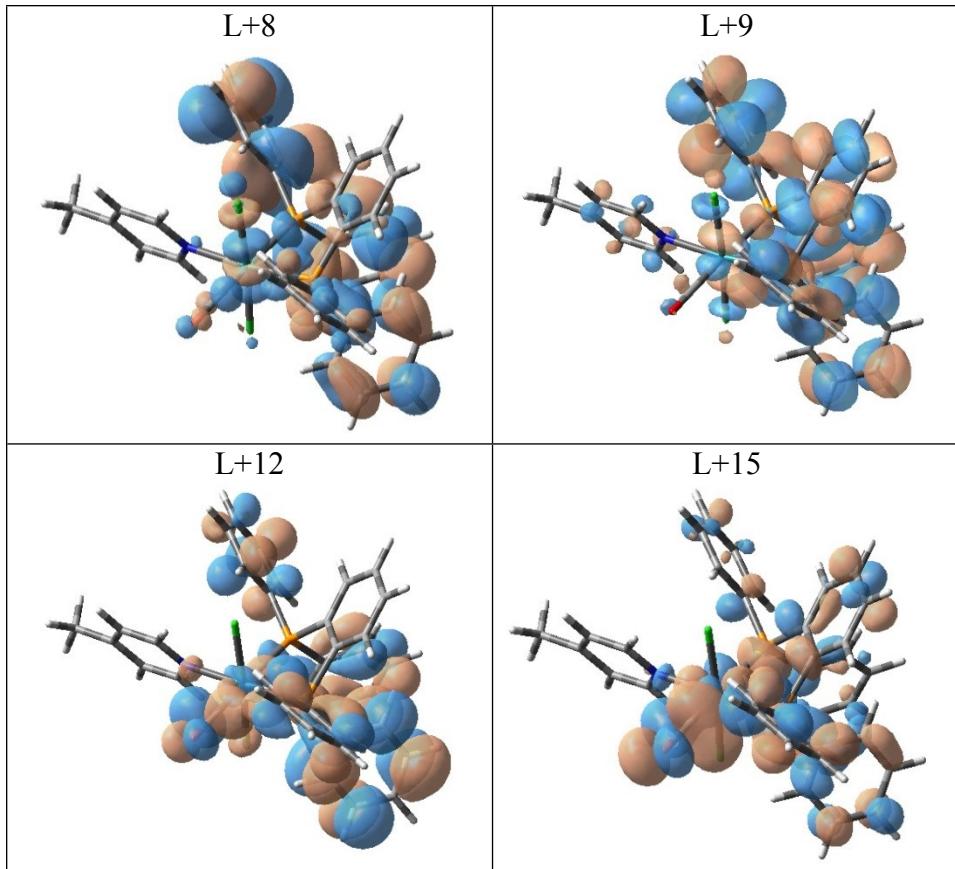
Fig. S7 Contour plots of selected molecular orbitals of [Ru(dppbz)(CO)(4-picoline)Cl$_2$].

Table S12   Computed parameters from TDDFT calculations on [Ru(dppbz)$_2$Cl$_2$] for electronic spectral properties in dichloromethane solution.

Excited state	Composition	CI value	E(eV)	Oscillator strength (f)	λ_{theo} (nm)	Assignment	λ_{exp} (nm)
1	H → L+2	0.70500	3.6379	0.0016	340.81	MLCT/LLCT	370
2	H-2 → L+1	0.67116	4.1330	0.1517	299.99	ILCT/LMCT/LLCT	313
	H-2 → L+4	0.12039				ILCT/LLCT	
3	H-5 → L	0.10891	4.4365	0.2226	279.47	ILCT/LMCT	276
	H-4 → L	0.68388				LLCT/ILCT/LMCT	

Table S13   Compositions of the molecular orbitals of [Ru(dppbz)$_2$Cl$_2$] associated with the electronic spectral transitions.

to	% Contribution of fragments		
	Ru	dppbz	Cl
HOMO(H)	61	5	34
H-2	2	62	36
H-3	81	19	0
H-4	1	32	67
H-5	6	88	6
LUMO(L)	22	78	0
L+1	21	71	8
L+2	1	99	0
L+4	2	98	0

HOMO (H)	LUMO (L)
H-2	L+1
H-3	L+2
H-4	L+4
H-5	
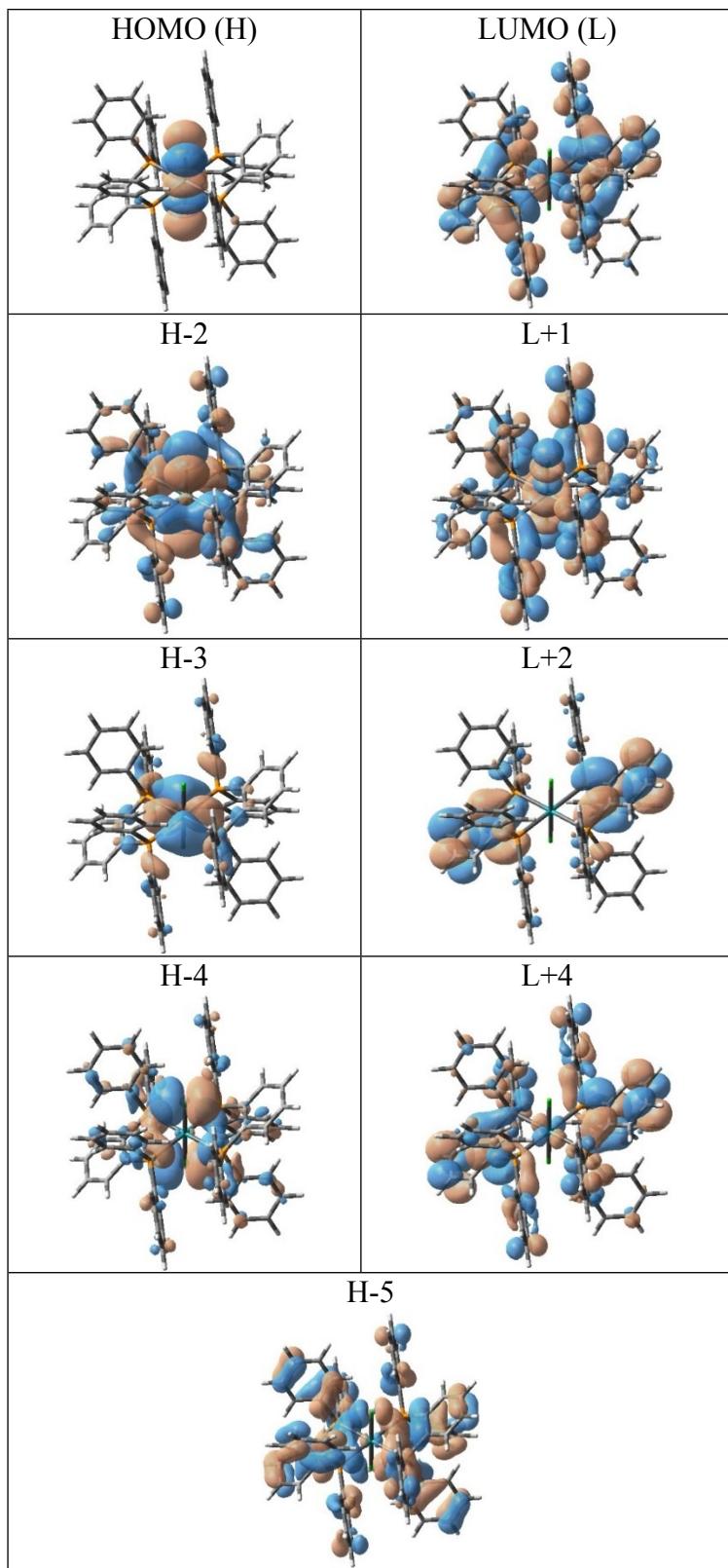
**Fig. S8**   Contour plots of selected molecular orbitals of [Ru(dppbz)$_2$Cl$_2$].

Table S14   Computed parameters from TDDFT calculations on [Ru(dppbz)(q)$_2$] for electronic spectral properties in dichloromethane solution.

Excited state	Composition	CI value	E(eV)	Oscillator strength (f)	λ_{theo} (nm)	Assignment	λ_{exp} (nm)
1	H-2 → L	0.13894	2.6380	0.0382	669.99	ILCT/MLCT	686
	H → L	0.66941				ILCT/MLCT	
2	H → L+1	0.68746	2.6806	0.0616	462.53	ILCT/MLCT	475
3	H-2 → L	0.55180	3.4049	0.0824	364.13	MLCT/ILCT	366
	H-1 → L+3	0.39384				LLCT/MLCT	
	H-1 → L+4	0.13598				ILCT/LLCT/MLCT /LMCT	
4	H-15 → L	0.28846	5.0175	0.1134	247.11	ILCT/LLCT/MLCT	248
	H-12 → L+1	0.15798				LLCT	
	H-11 → L	0.19934				LLCT	
	H-9 → L+1	0.18309				LLCT	
	H-8 → L	0.24883				ILCT/LLCT	
	H-7 → L+1	0.36831				ILCT/LLCT	
	H-3 → L+10	0.14209				LLCT/MLCT	
	H → L+16	0.13248				ILCT/MLCT	

Table 15   Compositions of the molecular orbitals of [Ru(dppbz)(q)$_2$] associated with the electronic spectral transitions.

Molecular orbital	% Contribution of fragments		
	Ru	dppbz	q
HOMO(H)	28	2	70
H-1	25	2	73
H-2	68	7	25
H-3	48	6	46
H-7	0	9	91
H-8	5	73	22
H-9	0	99	1
H-11	0	94	6
H-12	0	96	4
H-15	11	18	71
LUMO(L)	3	5	92
L+1	1	1	98
L+3	1	98	1
L+4	13	82	5
L+10	1	92	7
L+16	3	2	95

HOMO (H)	LUMO (L)
H-1	L+1
H-2	L+3
H-3	L+4

H-7	L+10
H-8	L+16
H-9	H-11
H-12	H-15
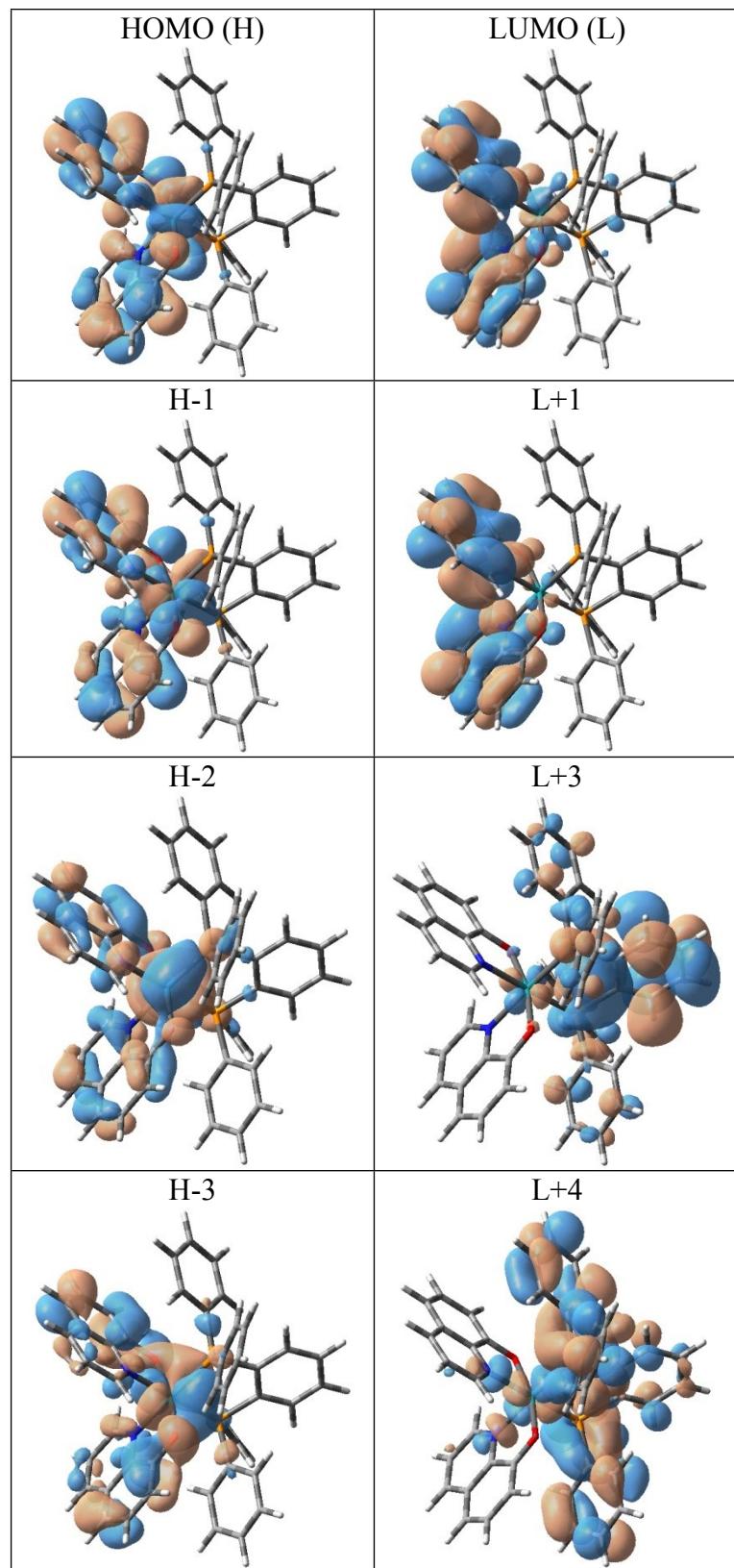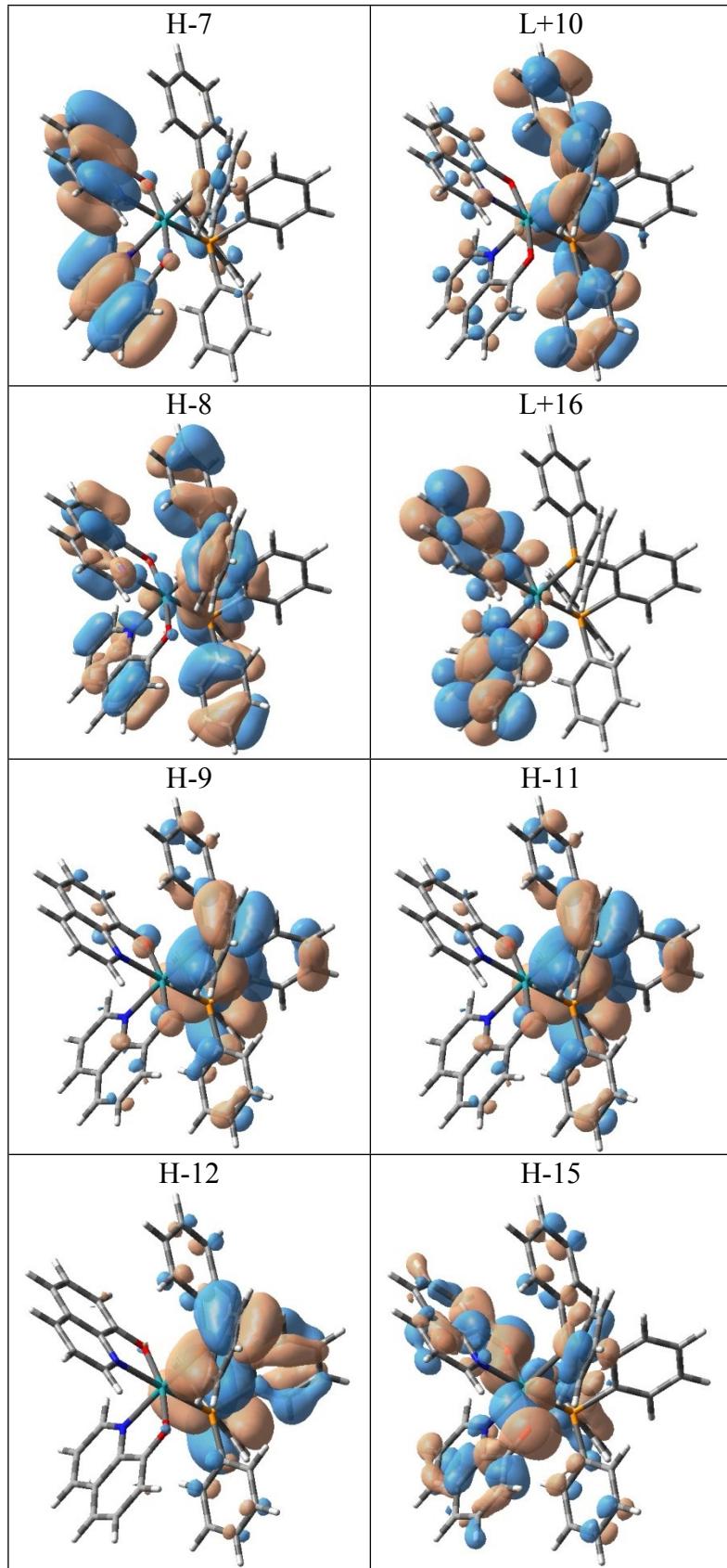
**Fig. S9** Contour plots of selected molecular orbitals of [Ru(dppbz)(q)$_2$].

Table S16   Computed parameters from TDDFT calculations on [Ru(dppbz)(pic)₂] for electronic spectral properties in dichloromethane solution.

Excited state	Composition	CI value	E(eV)	Oscillator strength (f)	λ_{theo} (nm)	Assignment	λ_{exp} (nm)
1	H-1 → L	0.10339	2.9754	0.0121	416.70	MLCT/ILCT	432
	H → L	0.65840				MLCT/ILCT	
2	H-2 → L+1	0.59390	3.6217	0.1081	342.34	MLCT/ILCT/LLCT	343
	H-1 → L+2	0.12226				LLCT/MLCT	
	H-1 → L+3	0.13900				ILCT/LLCT/MLCT	
	H → L+2	0.11525				LLCT/MLCT	
	H → L+4	0.24835				ILCT/LLCT/MLCT	
3	H-4 → L+3	0.10634	4.8828	0.0265	253.92	ILCT/LLCT	259
	H-3 → L+2	0.44126				LLCT	
	H-3 → L+3	0.19380				ILCT/LLCT	
	H-2 → L+8	0.12962				ILCT/LLCT/MLCT	
	H-2 → L+14	0.11793				ILCT/LLCT/MLCT /LMCT	
	H-1 → L+13	0.23401				LLCT/MLCT	
	H-1 → L+15	0.20847				ILCT/LLCT/MLCT /LMCT	
	H → L+15	0.12474				ILCT/LLCT/MLCT /LMCT	

Table S17   Compositions of the molecular orbitals of [Ru(dppbz)(pic)₂] associated with the electronic spectral transitions.

Molecular orbital	% Contribution of fragments		
	Ru	dppbz	pic
HOMO(H)	72	4	24
H-1	69	6	25
H-2	74	12	14
H-3	2	4	94
H-4	3	3	94
LUMO(L)	1	0	99
L+1	4	4	92
L+2	2	97	1
L+3	1	83	16
L+4	1	17	82
L+8	8	88	4
L+13	1	99	0
L+14	55	27	18
L+15	36	54	10

| HOMO (H)	LUMO (L)
H-1	L+1
H-2	L+2
H-3	L+3

H-4

L+4

L+8

L+13

L+14

L+15
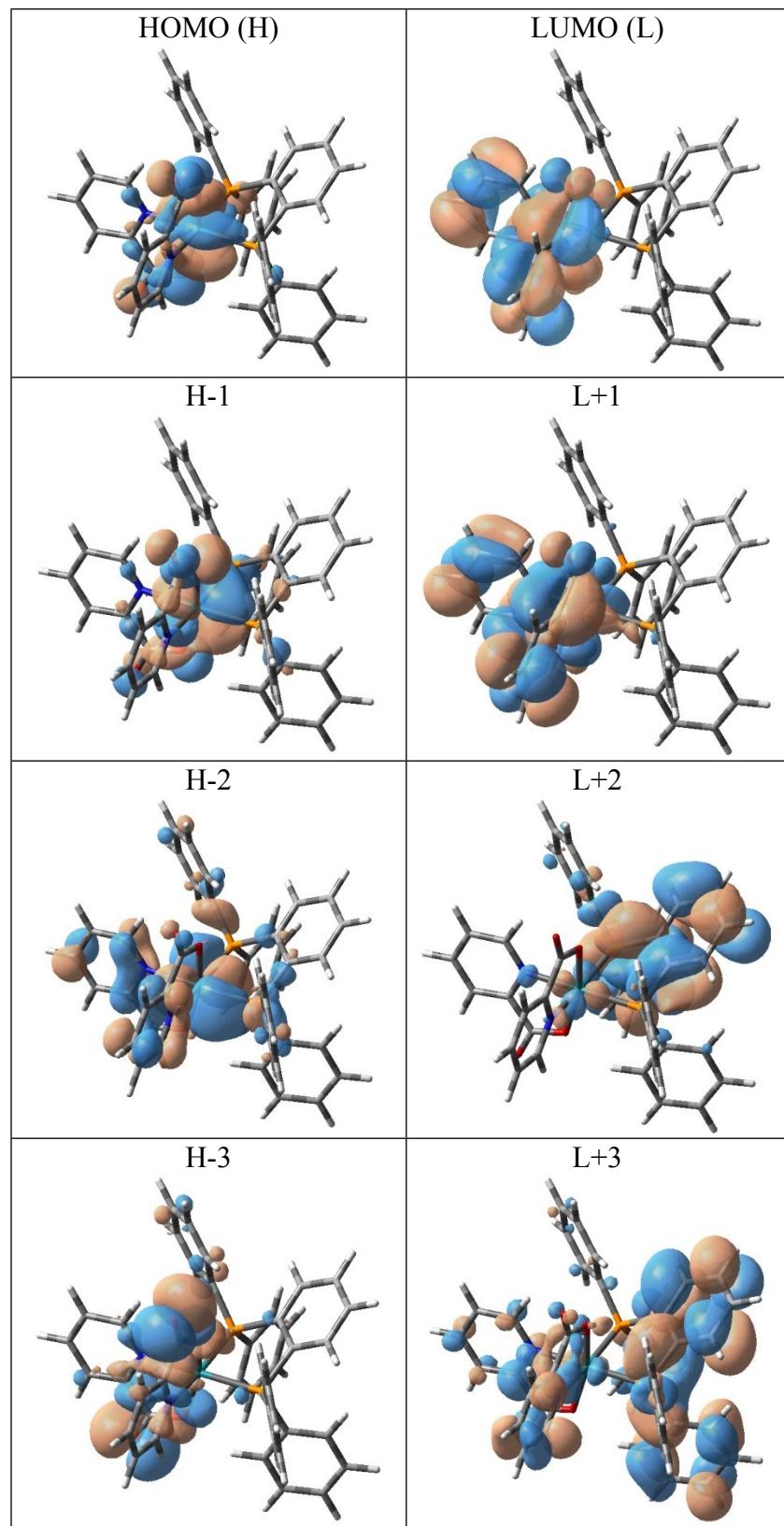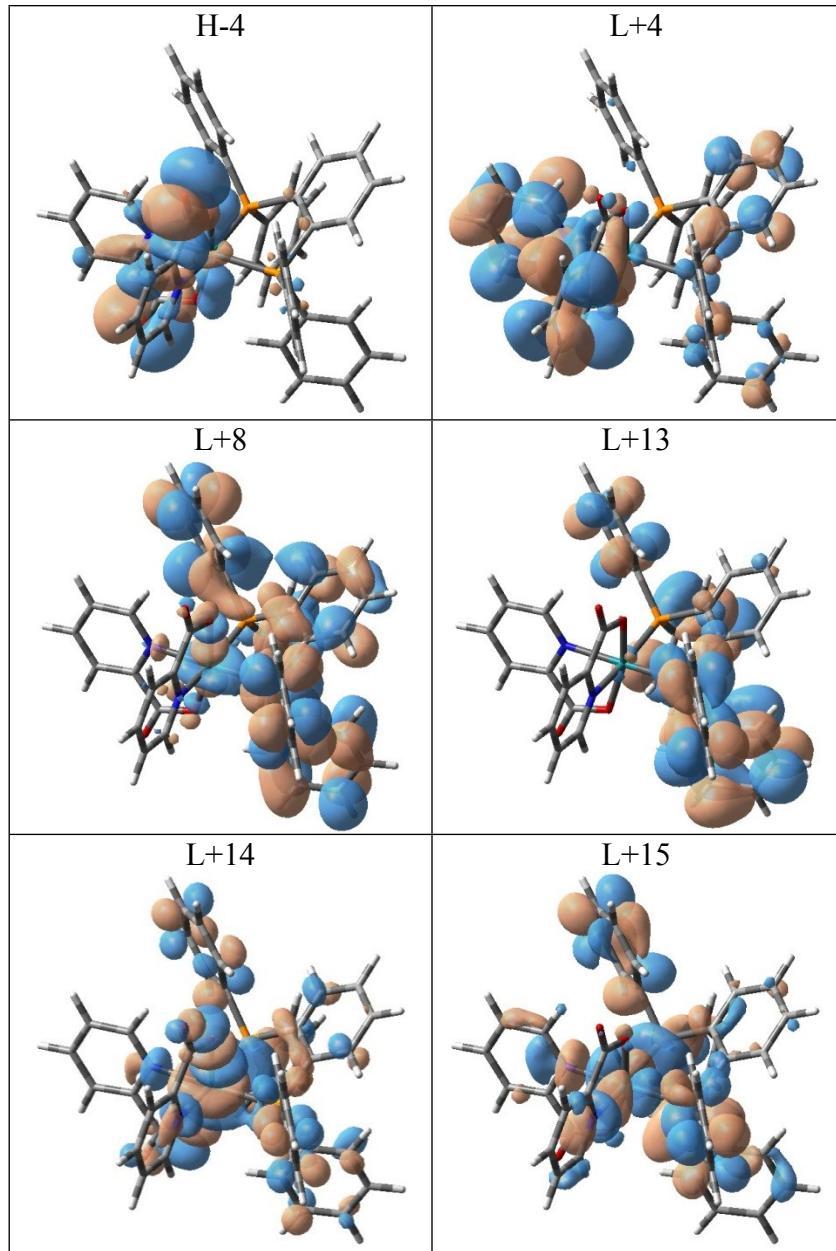
Fig. S10   Contour plots of selected molecular orbitals of [Ru(dppbz)(pic)₂].

Table S18. Screening of experimental conditions.[a]

Cl—◯—CHO $\xrightarrow[\text{solvent, base}]{\text{catalyst}^b}$ Cl—◯—CH$_2$OH
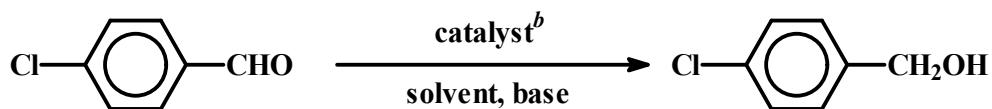
Entry	Solvent	Mole % of catalyst	Base	Temperature, °C	Time, h	Yield[c] %
1	1-propanol	0.02	KO^{t}Bu	95	6	99
2	1-propanol	0.01	KO^{t}Bu	95	6	68
3	1-propanol	0.01	KO^{t}Bu	95	10	62
4	1-propanol	0.02	KO^{t}Bu	95	5	89
5	1-propanol	-	KO^{t}Bu	95	6	NO[d]
6	1-propanol	0.02	-	95	6	NO[d]
7	1-propanol	0.02	KOH	95	6	16
8	1-propanol	0.02	K$_3$PO$_4$	95	6	NO[d]
9	1-propanol	0.02	KO^{t}Bu	50	6	32
10	2-propanol	0.02	KO^{t}Bu	80	6	85
11	ethanol	0.02	KO^{t}Bu	75	6	63

[a] Reaction conditions: 4-chlorobenzaldehyde (1.0 mmol), base (0.2 mol%), solvent (4.0 mL).
[b] Catalyst: [Ru(dppbz)(CO)$_2$Cl$_2$].
[c] Yields are determined by GCMS based on the quantity of substrate remaining after the reaction. Besides the substrate and the reported product, no other species was detected in any of the reactions.
[d] Not observed.

Table S19. Screening of experimental conditions.[a]
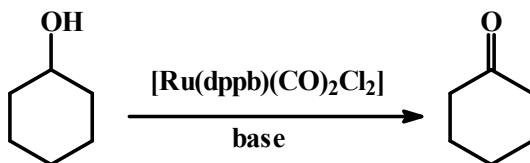
Entry	Solvent	Mole % of catalyst	Base	Temperature, °C	Time, h	Yeild[b], %
1	Toluene/Acetone	0.1	KO^{t}Bu	100	6	91
2	Toluene/Acetone	-	KO^{t}Bu	100	6	NO[c]
3	Toluene/Acetone	0.1	KO^{t}Bu	100	4	69
4	Toluene/Acetone	0.05	KO^{t}Bu	100	6	41
5	Toluene/Acetone	0.2	KO^{t}Bu	100	6	94
6	Toluene/Acetone	0.1	KO^{t}Bu	100	8	63
7	Toluene/Acetone	0.1	-	100	6	NO[c]
8	Toluene/Acetone	0.1	KOH	100	6	6
9	Toluene/Acetone	0.1	K$_3$PO$_4$	100	6	NO[c]
10	Toluene/Acetone	0.1	CsCO$_3$	100	6	5
11	Toluene/Acetone	0.1	KO^{t}Bu	60	6	39
12	Toluene	0.1	KO^{t}Bu	100	6	7
13	Acetone	0.1	KO^{t}Bu	100	6	68

[a] Reaction conditions: cyclohexanol (1.0 mmol), solvent (5.0 mL), base (0.25 mol%).
[b] Yields are determined by GCMS based on the quantity of substrate remaining after the reaction. Besides the substrate and the reported product, no other species was detected in any of the reactions.
[c] Not observed.

Table S20. Screening of experimental conditions.[a]
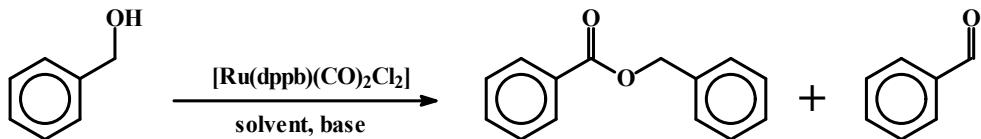
Entry	Solvent	Mole % of catalyst	Base	Temp-erature, °C	Time, h	Yield[b], (ester) %	Yield[b], (aldehyde) %
1	3:2 Toluene-Acetone	0.1	KOtBu	100	6	75	10
2	3:2 Toluene-Acetone	0.1	KOtBu	100	8	75	12
3	3:2 Toluene-Acetone	0.1	KOtBu	100	4	58	16
4	3:2 Toluene-Acetone	0.2	KOtBu	100	6	78	9
5	3:2 Toluene-Acetone	0.1	KOtBu	60	6	36	7
6	3:2 Toluene-Acetone	-	KOtBu	100	6	NO[c]	NO[c]
7	3:2 Toluene-Acetone	0.1	-	100	6	NO[c]	NO[c]
8	3:2 Toluene-Acetone	0.1	KOH	100	6	NO[c]	4
9	3:2 Toluene-Acetone	0.1	K_3PO_4	100	6	NO[c]	NO[c]
10	3:2 Toluene-Acetone	0.1	$CsCO_3$	100	6	NO[c]	NO[c]
11	Toluene	0.1	KOtBu	100	6	9	NO[c]
12	Acetone	0.1	KOtBu	100	6	48	16

[a] Reaction conditions: Benzyl alcohol (1.0 mmol), solvent (5.0 mL), base (0.25 mol%).
[b] Yields are determined by GCMS based on the quantity of substrate remaining after the reaction. Besides the substrate and the reported product(s), no other species was detected in any of the reactions.
[c] Not observed.

Table S21. Crystallographic data and structure refinement parameters

	[Ru(dppbz)(CO)(dmso)Cl$_2$]	[Ru(dppbz)$_2$Cl$_2$]	[Ru(dppbz)(q)$_2$]	[Ru(dppbz)(pic)$_2$]
empirical formula	C$_{33}$H$_{30}$O$_2$P$_2$SCl$_2$Ru	C$_{60}$H$_{48}$O$_2$P$_4$Cl$_2$Ru	C$_{48}$H$_{36}$N$_2$O$_2$P$_2$Ru	C$_{42}$H$_{32}$N$_2$O$_4$P$_2$Ru·C$_7$H$_8$
formula weight	724.55	1064.83	835.80	883.84
crystal system	triclinic	triclinic	monoclinic	triclinic
space group	P$\bar{1}$	P$\bar{1}$	P2$_1$/n	P$\bar{1}$
a (Å)	9.718(10)	10.5247(4)	11.5311(5)	10.0627(4)
b (Å)	10.552(12)	11.6210(4)	21.0156(8)	10.8128(4)
c (Å)	17.40(2)	12.8705(2)	16.2155(6)	20.1657(8)
α (°)	88.50(4)	86.888(2)	90	76.224(2)
β (°)	82.77(4)	77.258(2)	94.246(2)	79.050(3)
γ (°)	64.17(3)	80.961(2)	90	84.212(3)
V (Å^3)	1592(3)	1516.01(9)	3918.8(3)	2088.67(14)
Z	2	1	4	2
F (000)	736	546	1712	908
crystal size (mm)	0.14 × 0.14 × 0.20	0.12 × 0.18 × 0.22	0.22 × 0.24 × 0.28	0.20 × 0.25 × 0.30
T (K)	293	273	296	296
μ (mm^{-1})	0.856	0.485	0.525	0.500
R1[a]	0.1183	0.0478	0.0597	0.0537
wR2[b]	0.2980	0.1437	0.1997	0.1518
GOF[c]	0.94	1.03	1.13	0.94

[a] R1 = $\Sigma ||F_o| - |F_c|| / \Sigma |F_o|$. [b] wR2 = $[\Sigma\{w(F_o^2 - F_c^2)^2\}/\Sigma\{w(F_o^2)\}]^{1/2}$. [c] GOF = $[\Sigma(w(F_o^2 - F_c^2)^2)/(M-N)]^{1/2}$, where M is the number of reflections and N is the number of parameters refined.