Supporting information

Excited state properties of a series of molecular photocatalysts investigated by time-dependent density functional theory

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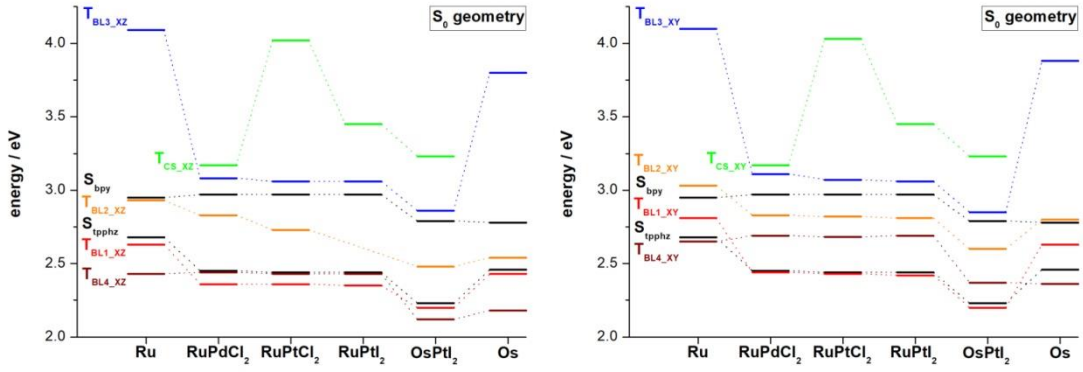

Figure S1. Excited states energy diagram calculated at the S_0 geometry.

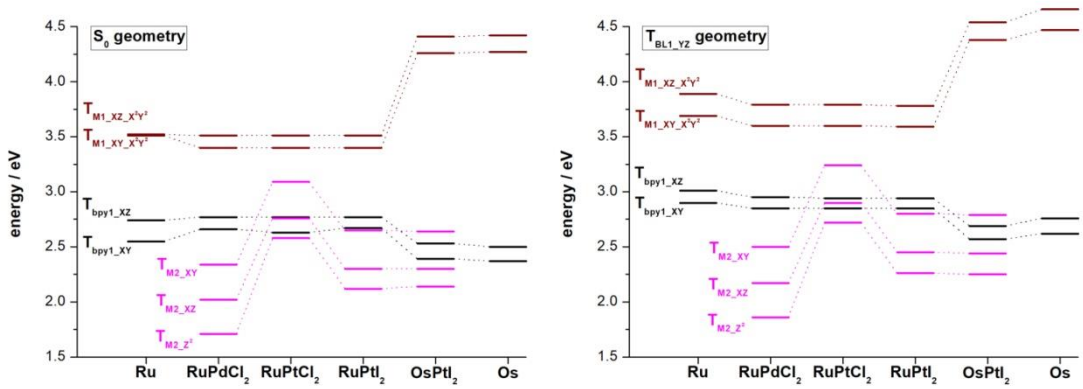

Figure S2. Excited states energy diagram calculated at the S_0 and T_{BL1_YZ} geometries.

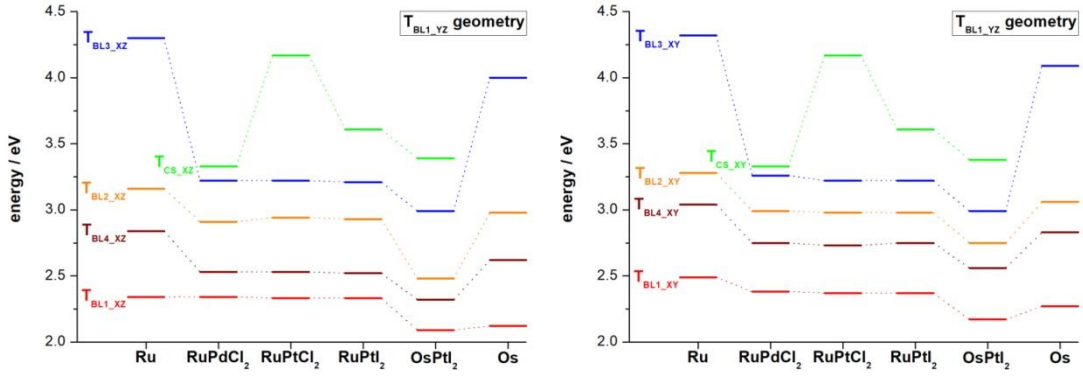

Figure S3. Excited states energy diagram calculated at the T_{BL1_YZ} geometry.

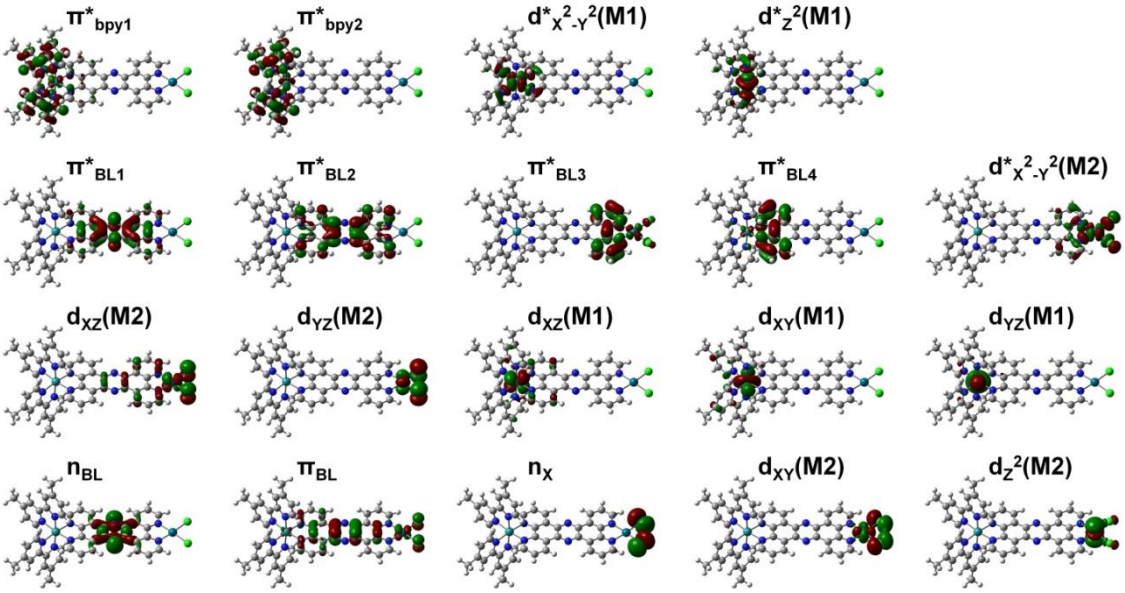

Figure S4. Frontier orbitals (**$RuPdCl_2$** at the S_0 geometry) and employed nomenclature.

Singlet-singlet transitions:

Table S1 Vertical excitation energies (VEE), wavelengths (λ), oscillator strengths (f) and singly-excited configurations of the main singlet excited states calculated at the S_0 geometry for **Ru**.

State	Transition	Weight (%)[a]	VEE (eV)	λ (nm)	f
S_6 (**S_{tpphz}**)	$d_{XZ}(Ru) \rightarrow \pi^*_{BL1}$	82	2.68	463	0.126
	$d_{XZ}(Ru) \rightarrow \pi^*_{BL4}$	11			
S_{11}	$d_{XZ}(Ru) \rightarrow \pi^*_{BL4}$	34	2.95	421	0.161
	$d_{XY}(Ru) \rightarrow \pi^*_{bpy2}$	25			
	$d_{XY}(Ru) \rightarrow \pi^*_{BL2}$	18			
S_{12} (**S_{bpy}**)	$d_{XY}(Ru) \rightarrow \pi^*_{bpy1}$	47	2.95	421	0.158
	$d_{XZ}(Ru) \rightarrow \pi^*_{bpy2}$	40			
S_{13}	$d_{XY}(Ru) \rightarrow \pi^*_{BL2}$	67	3.06	405	0.067
	$d_{XY}(Ru) \rightarrow \pi^*_{bpy2}$	29			
S_{14}	$d_{XZ}(Ru) \rightarrow \pi^*_{BL2}$	83	3.09	401	0.019
	$d_{XZ}(Ru) \rightarrow \pi^*_{bpy2}$	12			
S_{15}	$d_{XZ}(Ru) \rightarrow \pi^*_{bpy1}$	36	3.22	385	0.010
	$d_{XY}(Ru) \rightarrow \pi^*_{bpy2}$	27			

[a] Weights larger than 10%.

Table S2 Vertical excitation energies (VEE), wavelengths (λ), oscillator strengths (f) and singly-excited configurations of the main singlet excited states calculated at the S_0 geometry for **$RuPdCl_2$**.

State	Transition	Weight (%)[a]	VEE (eV)	λ (nm)	f
S_2 (**S_{tpphz}**)	$d_{XZ}(Ru) \rightarrow \pi^*_{BL1}$	96	2.45	506	0.058
S_{13}	$d_{XY}(Ru) \rightarrow \pi^*_{BL2}$	67	2.83	438	0.036
	$d_{XZ}(Ru) \rightarrow \pi^*_{BL4}$	26			
S_{15}	$d_{XZ}(Ru) \rightarrow \pi^*_{bpy1}$	41	2.86	434	0.062
	$d_{XZ}(Ru) \rightarrow \pi^*_{BL4}$	36			
	$d_{XY}(Ru) \rightarrow \pi^*_{BL2}$	16			
S_{16}	$d_{XZ}(Ru) \rightarrow \pi^*_{BL2}$	62	2.88	430	0.037
	$d_{XY}(Ru) \rightarrow \pi^*_{bpy1}$	20			
	$d_{XZ}(Ru) \rightarrow \pi^*_{bpy2}$	12			
S_{17}	$d_{XY}(Ru) \rightarrow \pi^*_{bpy2}$	40	2.93	423	0.205
	$d_{XZ}(Ru) \rightarrow \pi^*_{bpy1}$	23			
	$d_{XZ}(Ru) \rightarrow \pi^*_{BL4}$	21			
	$d_{XY}(Ru) \rightarrow \pi^*_{BL2}$	11			
S_{19} (**S_{bpy}**)	$d_{XZ}(Ru) \rightarrow \pi^*_{bpy2}$	52	2.97	418	0.142
	$d_{XY}(Ru) \rightarrow \pi^*_{bpy1}$	44			

[a] Weights larger than 10%.

Table S3 Vertical excitation energies (VEE), wavelengths (λ), oscillator strengths (f) and singly-excited configurations of the main singlet excited states calculated at the S_0 geometry for **$RuPtCl_2$**.

State	Transition	Weight (%)[a]	VEE (eV)	λ (nm)	f
S_2 (**S_{tpphz}**)	$d_{XZ}(Ru) \rightarrow \pi^*_{BL1}$	95	2.44	507	0.058
S_9	$d_{XY}(Ru) \rightarrow \pi^*_{BL2}$	75	2.82	439	0.022
	$d_{XZ}(Ru) \rightarrow \pi^*_{BL4}$	17			
S_{11}	$d_{XZ}(Ru) \rightarrow \pi^*_{BL4}$	44	2.86	434	0.088
	$d_{XZ}(Ru) \rightarrow \pi^*_{bpy1}$	39			
	$d_{XY}(Ru) \rightarrow \pi^*_{BL2}$	10			
S_{12}	$d_{XZ}(Ru) \rightarrow \pi^*_{BL2}$	46	2.88	431	0.034
	$d_{XY}(Ru) \rightarrow \pi^*_{bpy1}$	26			
	$d_{XZ}(Ru) \rightarrow \pi^*_{bpy2}$	19			
S_{15}	$d_{XY}(Ru) \rightarrow \pi^*_{bpy2}$	40	2.93	423	0.220
	$d_{XZ}(Ru) \rightarrow \pi^*_{bpy1}$	25			
	$d_{XZ}(Ru) \rightarrow \pi^*_{BL4}$	19			
S_{16} (**S_{bpy}**)	$d_{XZ}(Ru) \rightarrow \pi^*_{bpy2}$	51	2.97	417	0.144
	$d_{XY}(Ru) \rightarrow \pi^*_{bpy1}$	44			

[a] Weights larger than 10%.

Table S4 Vertical excitation energies (VEE), wavelengths (λ), oscillator strengths (f) and singly-excited configurations of the main singlet excited states calculated at the S_0 geometry for **RuPtI$_2$**.

State	Transition	Weight (%)[a]	VEE (eV)	λ (nm)	f
S_2 (**S_{tpphz}**)	$d_{XZ}(Ru) \rightarrow \pi^*_{BL1}$	95	2.44	508	0.065
S_{12}	$d_{XY}(Ru) \rightarrow \pi^*_{BL2}$	70	2.81	440	0.034
	$d_{XZ}(Ru) \rightarrow \pi^*_{BL4}$	21			
S_{16}	$d_{XZ}(Ru) \rightarrow \pi^*_{BL4}$	39	2.85	434	0.137
	$d_{XZ}(Ru) \rightarrow \pi^*_{bpy1}$	32			
	$d_{XY}(Ru) \rightarrow \pi^*_{BL2}$	16			
S_{17}	$d_{XZ}(Ru) \rightarrow \pi^*_{BL2}$	56	2.87	431	0.032
	$d_{XY}(Ru) \rightarrow \pi^*_{bpy1}$	22			
	$d_{XZ}(Ru) \rightarrow \pi^*_{bpy2}$	14			
S_{18}	$d_{XZ}(Pt) \rightarrow \pi^*_{BL1}$	81	2.88	430	0.129
S_{21}	$d_{XY}(Ru) \rightarrow \pi^*_{bpy2}$	39	2.93	423	0.128
	$d_{XZ}(Ru) \rightarrow \pi^*_{bpy1}$	23			
	$d_{XZ}(Ru) \rightarrow \pi^*_{BL4}$	19			
S_{22} (**S_{bpy}**)	$d_{XZ}(Ru) \rightarrow \pi^*_{bpy2}$	53	2.97	418	0.144
	$d_{XY}(Ru) \rightarrow \pi^*_{bpy1}$	42			

[a] Weights larger than 10%.

Table S5 Vertical excitation energies (VEE), wavelengths (λ), oscillator strengths (f) and singly-excited configurations of the main singlet excited states calculated at the S_0 geometry for **OsPtI$_2$**.

State	Transition	Weight (%)[a]	VEE (eV)	λ (nm)	f
S_3 (**S_{tpphz}**)	$d_{XZ}(Os) \rightarrow \pi^*_{BL1}$	93	2.23	555	0.061
S_8	$d_{XY}(Os) \rightarrow \pi^*_{BL4}$	79	2.49	498	0.014
S_9	$d_{XZ}(Os) \rightarrow \pi^*_{BL4}$	60	2.59	479	0.071
	$d_{XY}(Os) \rightarrow \pi^*_{BL2}$	22			
	$d_{XZ}(Os) \rightarrow \pi^*_{bpy1}$	10			
S_{10}	$d_{XY}(Os) \rightarrow \pi^*_{BL2}$	68	2.62	472	0.030
	$d_{XZ}(Os) \rightarrow \pi^*_{bpy1}$	13			
	$d_{XZ}(Os) \rightarrow \pi^*_{BL4}$	12			
S_{11}	$d_{XY}(Os) \rightarrow \pi^*_{bpy1}$	42	2.63	472	0.013
	$d_{XZ}(Os) \rightarrow \pi^*_{bpy2}$	32			
	$d_{XZ}(Os) \rightarrow \pi^*_{BL2}$	15			
S_{15}	$d_{XZ}(Os) \rightarrow \pi^*_{BL2}$	78	2.67	464	0.035
S_{17}	$d_{XY}(Os) \rightarrow \pi^*_{bpy2}$	46	2.77	447	0.312
	$d_{XZ}(Os) \rightarrow \pi^*_{bpy1}$	29			
	$d_{XZ}(Os) \rightarrow \pi^*_{BL4}$	14			
S_{18} (**S_{bpy}**)	$d_{XZ}(Os) \rightarrow \pi^*_{bpy2}$	60	2.79	443	0.157
	$d_{XY}(Os) \rightarrow \pi^*_{bpy1}$	34			
S_{21}	$d_{XZ}(Os) \rightarrow \pi^*_{BL3}$	82	2.84	436	0.011

[a] Weights larger than 10%.

Table S6 Vertical excitation energies (VEE), wavelengths (λ), oscillator strengths (f) and singly-excited configurations of the main singlet excited states calculated at the S_0 geometry for **Os**.

State	Transition	Weight (%)[a]	VEE (eV)	λ (nm)	f
S_6 (**S_{tpphz}**)	$d_{XZ}(Os) \rightarrow \pi^*_{BL1}$	80	2.46	503	0.124
	$d_{XZ}(Os) \rightarrow \pi^*_{BL4}$	14			
S_8	$d_{XY}(Os) \rightarrow \pi^*_{BL4}$	41	2.61	475	0.025
	$d_{XZ}(Os) \rightarrow \pi^*_{bpy2}$	31			
	$d_{XY}(Os) \rightarrow \pi^*_{bpy1}$	19			
S_9	$d_{YZ}(Os) \rightarrow \pi^*_{BL2}$	47	2.62	473	0.026
	$d_{XZ}(Os) \rightarrow \pi^*_{BL4}$	24			
	$d_{XZ}(Os) \rightarrow \pi^*_{bpy1}$	21			
S_{11}	$d_{XY}(Os) \rightarrow \pi^*_{BL2}$	30	2.78	446	0.132
	$d_{XY}(Os) \rightarrow \pi^*_{bpy2}$	28			
	$d_{XZ}(Os) \rightarrow \pi^*_{bpy1}$	19			
	$d_{XZ}(Os) \rightarrow \pi^*_{BL4}$	13			
S_{12} (**S_{bpy}**)	$d_{XZ}(Os) \rightarrow \pi^*_{bpy2}$	49	2.78	446	0.163
	$d_{XY}(Os) \rightarrow \pi^*_{bpy1}$	41			
S_{13}	$d_{XY}(Os) \rightarrow \pi^*_{BL2}$	60	2.85	435	0.130
	$d_{XY}(Os) \rightarrow \pi^*_{bpy2}$	30			
S_{14}	$d_{XZ}(Os) \rightarrow \pi^*_{BL2}$	92	2.88	430	0.026
S_{15}	$d_{XZ}(Os) \rightarrow \pi^*_{bpy1}$	47	3.06	404	0.031
	$d_{XY}(Os) \rightarrow \pi^*_{bpy2}$	26			

[a] Weights larger than 10%.

Singlet-triplet transitions:

Table S7 Vertical excitation energies (VEE), wavelengths (λ) and singly-excited configurations of the main triplet excited states calculated at the S_0 geometry for **Ru**.

State	Transition	Weight (%)	VEE (eV)	λ (nm)
T_1 ($\mathbf{T_{BL4\_YZ}}$)	$d_{YZ}(Ru) \rightarrow \pi^*_{BL4}$ $d_{YZ}(Ru) \rightarrow \pi^*_{bpy1}$ $d_{YZ}(Ru) \rightarrow \pi^*_{BL1}$	34 26 20	2.32	533
T_2 ($\mathbf{T_{BL4\_XZ}}$)	$d_{XZ}(Ru) \rightarrow \pi^*_{bpy1}$ $d_{XZ}(Ru) \rightarrow \pi^*_{BL4}$	42 33	2.43	510
T_3 ($\mathbf{T_{bpy2\_YZ}}$)	$d_{YZ}(Ru) \rightarrow \pi^*_{bpy2}$	76	2.46	503
T_4 ($\mathbf{T_{bpy1\_YZ}}$)	$d_{YZ}(Ru) \rightarrow \pi^*_{bpy1}$ $d_{YZ}(Ru) \rightarrow \pi^*_{BL4}$	56 25	2.48	499
T_5 ($\mathbf{T_{bpy1\_XY}}$)	$d_{YZ}(Ru) \rightarrow \pi^*_{BL1}$ $d_{XY}(Ru) \rightarrow \pi^*_{bpy1}$ $d_{XY}(Ru) \rightarrow \pi^*_{BL4}$ $d_{XY}(Ru) \rightarrow \pi^*_{BL1}$	23 20 15 10	2.55	487
T_6 ($\mathbf{T_{bpy2\_XY}}$)	$d_{XY}(Ru) \rightarrow \pi^*_{bpy2}$ $d_{XZ}(Ru) \rightarrow \pi^*_{BL1}$ $d_{XZ}(Ru) \rightarrow \pi^*_{BL4}$	57 16 10	2.59	479
T_7 ($\mathbf{T_{BL1\_YZ}}$)	$d_{YZ}(Ru) \rightarrow \pi^*_{BL1}$ $d_{YZ}(Ru) \rightarrow \pi^*_{BL4}$ $d_{XY}(Ru) \rightarrow \pi^*_{BL1}$ $d_{XY}(Ru) \rightarrow \pi^*_{bpy1}$	37 16 14 12	2.61	475
T_8 ($\mathbf{T_{BL1\_XZ}}$)	$d_{XZ}(Ru) \rightarrow \pi^*_{BL1}$ $\pi_{BL} \rightarrow \pi^*_{BL1}$ $d_{XY}(Ru) \rightarrow \pi^*_{bpy2}$	55 13 10	2.63	470
T_9 ($\mathbf{T_{BL4\_XY}}$)	$d_{XY}(Ru) \rightarrow \pi^*_{BL4}$ $d_{XY}(Ru) \rightarrow \pi^*_{bpy1}$ $d_{XZ}(Ru) \rightarrow \pi^*_{bpy2}$ $d_{XY}(Ru) \rightarrow \pi^*_{BL1}$	28 26 23 12	2.65	468
T_{10}	$\pi_{BL}[201] \rightarrow \pi^*_{BL1}$ $d_{YZ}(Ru) \rightarrow \pi^*_{BL4}$ $\pi_{BL} \rightarrow \pi^*_{BL2}$ $d_{YZ}(Ru) \rightarrow \pi^*_{BL1}$	28 12 10 10	2.67	463
T_{11} ($\mathbf{T_{bpy1\_XZ}}$)	$d_{XZ}(Ru) \rightarrow \pi^*_{bpy1}$ $d_{XZ}(Ru) \rightarrow \pi^*_{BL4}$	47 26	2.74	452
T_{12} ($\mathbf{T_{bpy2\_XZ}}$)	$d_{XZ}(Ru) \rightarrow \pi^*_{bpy2}$ $d_{XY}(Ru) \rightarrow \pi^*_{bpy1}$	46 25	2.77	447
T_{13} ($\mathbf{T_{BL1\_XY}}$)	$d_{XY}(Ru) \rightarrow \pi^*_{BL1}$ $d_{XY}(Ru) \rightarrow \pi^*_{BL4}$	49 30	2.81	441
T_{14} ($\mathbf{T_{BL2\_YZ}}$)	$d_{YZ}(Ru) \rightarrow \pi^*_{BL2}$	71	2.83	437
T_{15}	$\pi_{BL} \rightarrow \pi^*_{BL1}$ $d_{XZ}(Ru) \rightarrow \pi^*_{BL1}$	70 14	2.92	425
T_{16} ($\mathbf{T_{BL2\_XZ}}$)	$d_{XZ}(Ru) \rightarrow \pi^*_{BL2}$ $\pi_{BL}[201] \rightarrow \pi^*_{BL1}$	55 17	2.93	422
T_{17} ($\mathbf{T_{IL}}$)	$n_{BL} \rightarrow \pi^*_{BL1}$	83	2.99	414
T_{18} ($\mathbf{T_{BL2\_XY}}$)	$d_{XY}(Ru) \rightarrow \pi^*_{BL2}$	83	3.03	409
T_{19} ($\mathbf{T_{Ru\_YZ\_Z^2}}$)	$d_{YZ}(Ru) \rightarrow d^*_{Z^2}(Ru)$ $d_{YZ}(Ru) \rightarrow \pi^*_{bpy}[223]$	68 13	3.16	391
T_{20} ($\mathbf{T_{Ru\_YZ\_X^2Y^2}}$)	$d_{YZ}(Ru) \rightarrow d^*_{X^2-Y^2}(Ru)$	58	3.18	390
T_{21}	$\pi_{bpy}[198] \rightarrow \pi^*_{bpy2}$ $\pi_{bpy}[197] \rightarrow \pi^*_{bpy1}$ $\pi_{bpy}[197] \rightarrow \pi^*_{BL4}$	30 24 11	3.21	385
T_{22}	$\pi_{bpy}[197] \rightarrow \pi^*_{bpy2}$ $\pi_{bpy}[198] \rightarrow \pi^*_{bpy1}$ $d_{YZ}(Ru) \rightarrow d^*_{X^2-Y^2}(Ru)$	22 20 19	3.22	385
T_{23}	$\pi_{BL}[195] \rightarrow \pi^*_{BL1}$ $\pi_{BL}[195] \rightarrow \pi^*_{BL4}$	32 10	3.29	376

T_{24}	$\pi_{BL} \rightarrow \pi^*_{BL2}$ $\pi_{BL}[201] \rightarrow \pi^*_{BL1}$	54 23	3.30	376
T_{25} ($T_{Ru\_XY\_Z^2}$)	$d_{XY}(Ru) \rightarrow d^*_{Z^2}(Ru)$ $d_{XZ}(Ru) \rightarrow d^*_{X^2-Y^2}(Ru)$	48 30	3.41	364
T_{26}	$\pi_{BL}[201] \rightarrow \pi^*_{BL2}$ $\pi_{BL} \rightarrow \pi^*_{BL4}$	36 33	3.50	354
T_{27} ($T_{Ru\_XY\_X^2Y^2}$)	$d_{XY}(Ru) \rightarrow d^*_{X^2-Y^2}(Ru)$ $d_{XZ}(Ru) \rightarrow d^*_{Z^2}(Ru)$	37 35	3.51	352
T_{28} ($T_{Ru\_XZ\_X^2Y^2}$)	$d_{XZ}(Ru) \rightarrow d^*_{X^2-Y^2}(Ru)$ $d_{XY}(Ru) \rightarrow d^*_{Z^2}(Ru)$	50 25	3.52	352
T_{29}	$\sigma_{BL}[199] \rightarrow \pi^*_{BL1}$	87	3.55	349
T_{30}	$\pi_{BL}[201] \rightarrow \pi^*_{BL3}$ $\pi_{BL}[195] \rightarrow \pi^*_{BL4}$ $\pi_{BL}[201] \rightarrow \pi^*_{BL4}$	40 14 13	3.55	348
T_{33} ($T_{Ru\_XZ\_Z^2}$)	$d_{XY}(Ru) \rightarrow d^*_{X^2-Y^2}(Ru)$ $d_{XZ}(Ru) \rightarrow d^*_{Z^2}(Ru)$	37 32	3.59	345
T_{47} (T_{BL3_YZ})	$d_{YZ}(Ru) \rightarrow \pi^*_{BL3}$	98	3.93	315
T_{59} (T_{BL3_XZ})	$d_{XZ}(Ru) \rightarrow \pi^*_{BL3}$	69	4.09	302
T_{60} (T_{BL3_XY})	$d_{XY}(Ru) \rightarrow \pi^*_{BL3}$	98	4.10	302

[a] Weights larger than 10%.

Table S8 Vertical excitation energies (VEE), wavelengths (λ) and singly-excited configurations of the main triplet excited states calculated at the S_0 geometry for **$RuPdCl_2$**.

State	Transition	Weight (%)	VEE (eV)	λ (nm)
T_1 ($T_{Pd\_Z^2}$)	d_{Z^2}(Pd) → $d^*_{X^2-Y^2}$(Pd)	80	1.71	724
	d_{Z^2}(Pd) → π^*_{BL3}	18		
T_2 (T_{Pd_YZ})	d_{YZ}(Pd) → $d^*_{X^2-Y^2}$(Pd)	70	1.87	662
	d_{YZ}(Pd) → π^*_{BL3}	16		
T_3 (T_{Pd_XZ})	d_{XZ}(Pd) → $d^*_{X^2-Y^2}$(Pd)	61	2.02	614
	d_{XZ}(Pd) → π^*_{BL3}	14		
T_4 (**T_{BL1_YZ}**)	d_{YZ}(Ru) → π^*_{BL1}	59	2.23	554
	d_{YZ}(Ru) → π^*_{BL4}	27		
T_5 (T_{Pd_XY})	d_{XY}(Pd) → $d^*_{X^2-Y^2}$(Pd)	70	2.34	529
	d_{XY}(Pd) → π^*_{BL3}	16		
T_6 (**T_{BL1_XZ}**)	d_{XZ}(Ru) → π^*_{BL1}	54	2.36	524
	d_{XZ}(Ru) → π^*_{BL4}	31		
	d_{XZ}(Ru) → π^*_{bpy1}	10		
T_7 (**T_{BL4_YZ}**)	d_{YZ}(Ru) → π^*_{BL1}	36	2.38	521
	d_{YZ}(Ru) → π^*_{BL4}	24		
	d_{YZ}(Ru) → π^*_{bpy1}	10		
T_8 (**T_{BL4_XZ}**)	d_{XZ}(Ru) → π^*_{BL1}	37	2.44	508
	d_{XZ}(Ru) → π^*_{BL4}	24		
	d_{XZ}(Ru) → π^*_{bpy1}	13		
T_9 (**T_{BL1_XY}**)	d_{XY}(Ru) → π^*_{BL1}	76	2.44	507
T_{10} (**T_{bpy2_YZ}**)	d_{YZ}(Ru) → π^*_{bpy2}	79	2.49	498
T_{11} (**T_{bpy1_YZ}**)	d_{YZ}(Ru) → π^*_{bpy1}	66	2.51	493
	d_{YZ}(Ru) → π^*_{BL4}	17		
T_{12} (T_{BL})	d_{XZ}(Ru) → π^*_{BL2}	16	2.58	480
	d_{XY}(Ru) → π^*_{BL4}	15		
	d_{YZ}(Ru) → π^*_{BL4}	15		
	d_{XY}(Ru) → π^*_{bpy1}	13		
	d_{XY}(Ru) → π^*_{BL1}	11		
T_{13} (**T_{bpy2_XY}**)	d_{XY}(Ru) → π^*_{bpy2}	72	2.61	475
	d_{XZ}(Ru) → π^*_{BL4}	13		
T_{14} (T_{BL2_YZ})	d_{YZ}(Ru) → π^*_{BL2}	79	2.65	468
T_{15} (**T_{bpy1_XY}**)	d_{XY}(Ru) → π^*_{bpy1}	44	2.66	466
	d_{XZ}(Ru) → π^*_{bpy2}	14		
	d_{XZ}(Ru) → π^*_{BL2}	10		
T_{16} (**T_{BL4_XY}**)	d_{XY}(Ru) → π^*_{BL4}	61	2.69	461
T_{17} (**T_{bpy1_XZ}**)	d_{XZ}(Ru) → π^*_{bpy1}	55	2.77	447
	d_{XZ}(Ru) → π^*_{BL4}	15		
T_{18} (**T_{bpy2_XZ}**)	d_{XZ}(Ru) → π^*_{bpy2}	43	2.79	444
	d_{XY}(Ru) → π^*_{bpy1}	26		
T_{19} (T_{BL2_XZ})	d_{XZ}(Ru) → π^*_{BL2}	36	2.83	438
	π_{BL}[220] → π^*_{BL1}	17		
	d_{XZ}(Ru) → π^*_{bpy2}	14		
T_{20} (T_{BL2_XY})	d_{XY}(Ru) → π^*_{BL2}	82	2.83	437
T_{21} (T_{BL3_YZ})	d_{YZ}(Ru) → π^*_{BL3}	84	2.95	420
	d_{YZ}(Ru) → $d^*_{X^2-Y^2}$(Pd)	14		
T_{22} (**T_{MLCT}**)	d_{XZ}(Pd) → π^*_{BL1}	47	2.97	417
	π_{BL} → π^*_{BL1}	39		
T_{23} (**T_{IL}**)	n_{BL} → π^*_{BL1}	89	2.99	414
T_{24} (T_{CS_YZ})	d_{YZ}(Ru) → $d^*_{X^2-Y^2}$(Pd)	85	3.02	410
	d_{YZ}(Ru) → π^*_{BL3}	14		
T_{25} (T_{BL3_XZ})	d_{XZ}(Ru) → π^*_{BL3}	71	3.08	402
	d_{XZ}(Ru) → $d^*_{X^2-Y^2}$(Pd)	13		
T_{26}	d_{YZ}(Pd) → π^*_{BL3}	21	3.10	399
	π_{BL}[220] → π^*_{BL1}	13		
T_{27} (T_{BL3_XY})	d_{XY}(Ru) → π^*_{BL3}	82	3.11	398
	d_{XY}(Ru) → $d^*_{X^2-Y^2}$(Pd)	13		

T_{28} ($T_{Ru\_YZ\_X^2Y^2}$)	$d_{YZ}(Ru) \rightarrow d^*_{X^2-Y^2}(Ru)$	76	3.16	392
T_{29} (T_{CS_XZ})	$d_{XZ}(Ru) \rightarrow d^*_{X^2-Y^2}(Pd)$ $d_{XZ}(Ru) \rightarrow \pi^*_{BL3}$	82 16	3.17	391
T_{30} (T_{CS_XY})	$d_{XY}(Ru) \rightarrow d^*_{X^2-Y^2}(Pd)$ $d_{XY}(Ru) \rightarrow \pi^*_{BL3}$	85 14	3.17	390
T_{31} ($T_{Ru\_YZ\_Z^2}$)	$d_{YZ}(Ru) \rightarrow d^*_{Z^2}(Ru)$	53	3.18	389
T_{39} ($T_{Ru\_XY\_X^2Y^2}$)	$d_{XY}(Ru) \rightarrow d^*_{X^2-Y^2}(Ru)$ $d_{XZ}(Ru) \rightarrow d^*_{Z^2}(Ru)$	59 23	3.40	364
T_{43} ($T_{Ru\_XZ\_X^2Y^2}$)	$d_{XZ}(Ru) \rightarrow d^*_{X^2-Y^2}(Ru)$ $d_{XY}(Ru) \rightarrow d^*_{Z^2}(Ru)$	40 32	3.51	353
T_{44} ($T_{Ru\_XZ\_Z^2}$)	$d_{XZ}(Ru) \rightarrow d^*_{Z^2}(Ru)$ $d_{XY}(Ru) \rightarrow d^*_{X^2-Y^2}(Ru)$	49 24	3.52	352
T_{49} ($T_{Ru\_XY\_Z^2}$)	$d_{XZ}(Ru) \rightarrow d^*_{X^2-Y^2}(Ru)$ $d_{XY}(Ru) \rightarrow d^*_{Z^2}(Ru)$	42 36	3.58	346

[a] Weights larger than 10%.

Table S9 Vertical excitation energies (VEE), wavelengths (λ) and singly-excited configurations of the main triplet excited states calculated at the S_0 geometry for **$RuPtCl_2$**.

State	Transition	Weight (%)	VEE (eV)	λ (nm)
T_1 (T_{BL1_YZ})	$d_{YZ}(Ru) \rightarrow \pi^*_{BL1}$ $d_{YZ}(Ru) \rightarrow \pi^*_{BL4}$	61 26	2.23	556
T_2 (T_{BL1_XZ})	$d_{XZ}(Ru) \rightarrow \pi^*_{BL1}$ $d_{XZ}(Ru) \rightarrow \pi^*_{BL4}$	58 28	2.36	525
T_3 (T_{BL4_YZ})	$d_{YZ}(Ru) \rightarrow \pi^*_{BL1}$ $d_{YZ}(Ru) \rightarrow \pi^*_{BL4}$ $d_{YZ}(Ru) \rightarrow \pi^*_{bpy1}$	34 25 10	2.37	522
T_4 (T_{BL4_XZ})	$d_{XZ}(Ru) \rightarrow \pi^*_{BL1}$ $d_{XZ}(Ru) \rightarrow \pi^*_{BL4}$ $d_{XZ}(Ru) \rightarrow \pi^*_{bpy1}$	33 28 14	2.43	510
T_5 (T_{BL1_XY})	$d_{XY}(Ru) \rightarrow \pi^*_{BL1}$	77	2.43	509
T_6 (T_{bpy2_YZ})	$d_{YZ}(Ru) \rightarrow \pi^*_{bpy2}$	79	2.49	498
T_7 (T_{bpy1_YZ})	$d_{YZ}(Ru) \rightarrow \pi^*_{bpy1}$ $d_{YZ}(Ru) \rightarrow \pi^*_{BL4}$	68 15	2.51	493
T_8 (T_{Pt_YZ})	$d_{YZ}(Pt) \rightarrow d^*_{X^2-Y^2}(Pt)$	65	2.56	484
T_9	$d_{YZ}(Pt) \rightarrow d^*_{X^2-Y^2}(Pt)$ $d_{YZ}(Ru) \rightarrow \pi^*_{BL4}$ $d_{XZ}(Ru) \rightarrow \pi^*_{BL2}$	24 12 10	2.57	483
T_{10} ($T_{Pt\_Z^2}$)	$d_{Z^2}(Pt) \rightarrow d^*_{X^2-Y^2}(Pt)$	88	2.58	479
T_{11} (T_{bpy2_XY})	$d_{XY}(Ru) \rightarrow \pi^*_{bpy2}$ $d_{XZ}(Ru) \rightarrow \pi^*_{BL4}$	72 12	2.61	475
T_{12} (T_{bpy1_XY})	$d_{XY}(Ru) \rightarrow \pi^*_{bpy1}$ $d_{XY}(Ru) \rightarrow \pi^*_{BL4}$ $d_{YZ}(Pt) \rightarrow \pi^*_{BL3}$	30 13 12	2.63	471
T_{13} (T_{BL2_YZ})	$d_{YZ}(Ru) \rightarrow \pi^*_{BL2}$	78	2.64	470
T_{14} (T_{BL4_XY})	$d_{XY}(Ru) \rightarrow \pi^*_{BL4}$ $d_{XY}(Ru) \rightarrow \pi^*_{bpy1}$ $d_{XZ}(Ru) \rightarrow \pi^*_{bpy2}$	47 23 17	2.68	462
T_{15} (T_{BL2_XZ})	$d_{XZ}(Ru) \rightarrow \pi^*_{BL2}$ $d_{YZ}(Pt) \rightarrow \pi^*_{BL3}$	46 16	2.73	453
T_{16} (T_{Pt_XZ})	$d_{XZ}(Pt) \rightarrow d^*_{X^2-Y^2}(Pt)$	85	2.76	449
T_{17} (T_{bpy1_XZ})	$d_{XZ}(Ru) \rightarrow \pi^*_{bpy1}$ $d_{XZ}(Ru) \rightarrow \pi^*_{BL4}$ $d_{XY}(Ru) \rightarrow \pi^*_{BL2}$	54 13 10	2.77	448
T_{18} (T_{bpy2_XZ})	$d_{XZ}(Ru) \rightarrow \pi^*_{bpy2}$ $d_{XY}(Ru) \rightarrow \pi^*_{bpy1}$	56 24	2.80	442
T_{19} (T_{BL2_XY})	$d_{XY}(Ru) \rightarrow \pi^*_{BL2}$	78	2.82	439
T_{20}	$d_{XZ}(Pt) \rightarrow \pi^*_{BL3}$	75	2.84	437
T_{21} (T_{MLCT})	$d_{XZ}(Pt) \rightarrow \pi^*_{BL1}$ $\pi_{BL} \rightarrow \pi^*_{BL1}$	65 22	2.88	430
T_{22} (T_{BL3_YZ})	$d_{YZ}(Ru) \rightarrow \pi^*_{BL3}$	59	2.91	425
T_{23}	$d_{YZ}(Ru) \rightarrow \pi^*_{BL3}$ $\pi_{BL}[221] \rightarrow \pi^*_{BL1}$ $d_{YZ}(Pt) \rightarrow \pi^*_{BL1}$	39 12 12	2.92	425
T_{24}	$d_{Z^2}(Pt) \rightarrow \pi^*_{BL3}$ $d_{Z^2}(Pt) \rightarrow \pi^*_{BL1}$	52 30	2.93	423
T_{25} (T_{IL})	$n_{BL} \rightarrow \pi^*_{BL1}$ $\pi_{BL}[217] \rightarrow \pi^*_{BL1}$	76 12	2.99	414
T_{26}	$d_{YZ}(Pt) \rightarrow \pi^*_{BL1}$ $d_{YZ}(Pt) \rightarrow \pi^*_{BL3}$	55 26	3.01	412
T_{27} (T_{BL3_XZ})	$d_{XZ}(Ru) \rightarrow \pi^*_{BL3}$	94	3.06	404
T_{28} (T_{BL3_XY})	$d_{XY}(Ru) \rightarrow \pi^*_{BL3}$	98	3.07	403
T_{29} (T_{Pt_XY})	$d_{XY}(Pt) \rightarrow d^*_{X^2-Y^2}(Pt)$	92	3.09	401
T_{30} ($T_{Ru\_YZ\_X^2Y^2}$)	$d_{YZ}(Ru) \rightarrow d^*_{X^2-Y^2}(Ru)$	77	3.16	392
T_{32} ($T_{Ru\_YZ\_Z^2}$)	$d_{YZ}(Ru) \rightarrow d^*_{Z^2}(Ru)$	53	3.18	389
T_{40} ($T_{Ru\_XY\_X^2Y^2}$)	$d_{XY}(Ru) \rightarrow d^*_{X^2-Y^2}(Ru)$	59	3.40	364

	d_{XZ}(Ru) → $d^*_{Z^2}$(Ru)	22		
T_{43} ($T_{Ru\_XZ\_X^2Y^2}$)	d_{XZ}(Ru) → $d^*_{X^2-Y^2}$(Ru) d_{XY}(Ru) → $d^*_{Z^2}$(Ru)	38 33	3.51	353
T_{44} ($T_{Ru\_XZ\_Z^2}$)	d_{XZ}(Ru) → $d^*_{Z^2}$(Ru) d_{XY}(Ru) → $d^*_{X^2-Y^2}$(Ru)	47 23	3.52	352
T_{49} ($T_{Ru\_XY\_Z^2}$)	d_{XZ}(Ru) → $d^*_{X^2-Y^2}$(Ru) d_{XY}(Ru) → $d^*_{Z^2}$(Ru)	41 35	3.58	346
T_{66} (T_{CS_YZ})	d_{YZ}(Ru) → $d^*_{X^2-Y^2}$(Pt)	99	3.87	320
T_{75} (T_{CS_XZ})	d_{XZ}(Ru) → $d^*_{X^2-Y^2}$(Pt)	99	4.02	308
T_{77} (T_{CS_XY})	d_{XY}(Ru) → $d^*_{X^2-Y^2}$(Pt)	99	4.03	307

[a] Weights larger than 10%.

Table S10 Vertical excitation energies (VEE), wavelengths (λ) and singly-excited configurations of the main triplet excited states calculated at the S_0 geometry for **RuPtI$_2$**.

State	Transition	Weight (%)	VEE (eV)	λ (nm)
T_1 (T_{Pt_YZ})	$d_{YZ}(Pt) \rightarrow d^*_{X^2-Y^2}(Pt)$ $d_{Z^2}(Pt) \rightarrow d^*_{X^2-Y^2}(Pt)$ $d_{XY}(Pt) \rightarrow d^*_{X^2-Y^2}(Pt)$	47 24 18	2.11	586
T_2 ($T_{Pt\_Z^2}$)	$d_{YZ}(Pt) \rightarrow d^*_{X^2-Y^2}(Pt)$ $d_{Z^2}(Pt) \rightarrow d^*_{X^2-Y^2}(Pt)$ $d_{XY}(Pt) \rightarrow d^*_{X^2-Y^2}(Pt)$	35 31 24	2.12	584
T_3 (**T_{BL1_YZ}**)	$d_{YZ}(Ru) \rightarrow \pi^*_{BL1}$ $d_{YZ}(Ru) \rightarrow \pi^*_{BL4}$	61 25	2.23	555
T_4 (T_{Pt_XZ})	$d_{XZ}(Pt) \rightarrow d^*_{X^2-Y^2}(Pt)$ $n_I[205] \rightarrow d^*_{X^2-Y^2}(Pt)$	85 11	2.30	538
T_5 (**T_{BL1_XZ}**)	$d_{XZ}(Ru) \rightarrow \pi^*_{BL1}$ $d_{XZ}(Ru) \rightarrow \pi^*_{BL4}$	61 27	2.35	526
T_6 (**T_{BL4_YZ}**)	$d_{YZ}(Ru) \rightarrow \pi^*_{BL1}$ $d_{YZ}(Ru) \rightarrow \pi^*_{BL4}$	33 22	2.37	522
T_7 (**T_{BL1_XY}**)	$d_{XY}(Ru) \rightarrow \pi^*_{BL1}$	75	2.42	511
T_8 (**T_{BL4_XZ}**)	$d_{XZ}(Ru) \rightarrow \pi^*_{BL1}$ $d_{XZ}(Ru) \rightarrow \pi^*_{BL4}$ $d_{XZ}(Ru) \rightarrow \pi^*_{bpy1}$	31 31 14	2.43	510
T_9 (**T_{bpy2_YZ}**)	$d_{YZ}(Ru) \rightarrow \pi^*_{bpy2}$	80	2.50	496
T_{10} (**T_{bpy1_YZ}**)	$d_{YZ}(Ru) \rightarrow \pi^*_{bpy1}$ $d_{YZ}(Ru) \rightarrow \pi^*_{BL4}$	68 13	2.52	492
T_{11}	$d_{YZ}(Pt) \rightarrow \pi^*_{BL3}$ $d_{YZ}(Pt) \rightarrow \pi^*_{BL1}$ $d_{YZ}(Ru) \rightarrow \pi^*_{BL4}$ $\pi_{BL}[209] \rightarrow \pi^*_{BL1}$	17 17 16 10	2.55	486
T_{12}	$d_{XY}(Ru) \rightarrow \pi^*_{BL4}$ $d_{XY}(Ru) \rightarrow \pi^*_{bpy1}$ $d_{YZ}(Pt) \rightarrow \pi^*_{BL1}$ $d_{YZ}(Pt) \rightarrow \pi^*_{BL3}$	22 20 15 10	2.60	477
T_{13} (**T_{bpy2_XY}**)	$d_{XY}(Ru) \rightarrow \pi^*_{bpy2}$ $d_{XZ}(Ru) \rightarrow \pi^*_{BL4}$	74 12	2.60	476
T_{14} (T_{BL2_YZ})	$d_{YZ}(Ru) \rightarrow \pi^*_{BL2}$	80	2.65	468
T_{15} (T_{Pt_XY})	$d_{XY}(Pt) \rightarrow d^*_{X^2-Y^2}(Pt)$ $d_{Z^2}(Pt) \rightarrow d^*_{X^2-Y^2}(Pt)$	49 39	2.65	467
T_{16} (**T_{bpy1_XY}**)	$d_{XY}(Ru) \rightarrow \pi^*_{bpy1}$ $d_{XZ}(Ru) \rightarrow \pi^*_{bpy2}$ $d_{XY}(Ru) \rightarrow \pi^*_{BL4}$	42 18 16	2.67	465
T_{17} (**T_{BL4_XY}**)	$d_{XY}(Ru) \rightarrow \pi^*_{BL4}$ $d_{XZ}(Ru) \rightarrow \pi^*_{BL2}$ $d_{YZ}(Pt) \rightarrow \pi^*_{BL1}$	35 26 17	2.69	461
T_{18} (**T_{MLCT}**)	$n_I \rightarrow d^*_{X^2-Y^2}(Pt)$ $d_{XZ}(Pt) \rightarrow \pi^*_{BL3}$ $d_{XZ}(Pt) \rightarrow \pi^*_{BL1}$	33 32 26	2.75	451
T_{19}	$n_I \rightarrow d^*_{X^2-Y^2}(Pt)$ $d_{XZ}(Ru) \rightarrow \pi^*_{bpy1}$ $d_{XZ}(Pt) \rightarrow \pi^*_{BL1}$	34 26 13	2.76	448
T_{20} (**T_{bpy1_XZ}**)	$d_{XZ}(Ru) \rightarrow \pi^*_{bpy1}$ $n_I \rightarrow d^*_{X^2-Y^2}(Pt)$ $d_{XZ}(Pt) \rightarrow \pi^*_{BL1}$	28 26 11	2.77	448
T_{21}	$d_{YZ}(Pt) \rightarrow \pi^*_{BL1}$ $d_{YZ}(Pt) \rightarrow \pi^*_{BL3}$ $d_{XZ}(Ru) \rightarrow \pi^*_{BL2}$	36 21 13	2.78	446
T_{22} (**T_{bpy2_XZ}**)	$d_{XZ}(Ru) \rightarrow \pi^*_{bpy2}$ $d_{XY}(Ru) \rightarrow \pi^*_{bpy1}$	52 19	2.80	443
T_{23}	$n_I \rightarrow \pi^*_{BL1}$	92	2.81	440
T_{24} (T_{BL2_XY})	$d_{XY}(Ru) \rightarrow \pi^*_{BL2}$	67	2.81	440

T_{25}	$d_{XZ}(Pt) \rightarrow \pi^*_{BL3}$ $d_{XZ}(Pt) \rightarrow \pi^*_{BL1}$ $d_{XY}(Ru) \rightarrow \pi^*_{BL2}$	30 25 12	2.82	440
T_{26}	$d_{YZ}(Pt) \rightarrow \pi^*_{BL3}$ $\pi_{BL}[209] \rightarrow \pi^*_{BL1}$ $d_{XZ}(Ru) \rightarrow \pi^*_{BL2}$	27 26 19	2.88	430
T_{27}	$d_{Z^2}(Pt) \rightarrow \pi^*_{BL3}$ $d_{XY}(Pt) \rightarrow \pi^*_{BL3}$ $d_{Z^2}(Pt) \rightarrow \pi^*_{BL1}$ $d_{XY}(Pt) \rightarrow \pi^*_{BL1}$	32 25 20 17	2.89	429
T_{28} ($\mathbf{T_{BL3\_YZ}}$)	$d_{YZ}(Ru) \rightarrow \pi^*_{BL3}$	98	2.92	424
T_{29} ($\mathbf{T_{IL}}$)	$n_{BL} \rightarrow \pi^*_{BL1}$	87	2.99	415
T_{30}	$n_{I} \rightarrow \pi^*_{BL3}$	92	3.03	409
T_{32} ($\mathbf{T_{BL3\_XZ}}$)	$d_{XZ}(Ru) \rightarrow \pi^*_{BL3}$ $d_{YZ}(Pt) \rightarrow \pi^*_{BL2}$	86 10	3.06	405
T_{33} ($\mathbf{T_{BL3\_XY}}$)	$d_{XY}(Ru) \rightarrow \pi^*_{BL3}$	98	3.06	404
T_{38} ($\mathbf{T_{Ru\_YZ\_X^2Y^2}}$)	$d_{YZ}(Ru) \rightarrow d^*_{X^2-Y^2}(Ru)$	73	3.17	391
T_{40} ($\mathbf{T_{Ru\_YZ\_Z^2}}$)	$d_{YZ}(Ru) \rightarrow d^*_{Z^2}(Ru)$	50	3.19	389
T_{45} ($\mathbf{T_{CS\_YZ}}$)	$d_{YZ}(Ru) \rightarrow d^*_{X^2-Y^2}(Pt)$	99	3.31	374
T_{47} ($\mathbf{T_{Ru\_XY\_X^2Y^2}}$)	$d_{XY}(Ru) \rightarrow d^*_{X^2-Y^2}(Ru)$ $d_{XZ}(Ru) \rightarrow d^*_{Z^2}(Ru)$	58 22	3.40	364
T_{48} ($\mathbf{T_{CS\_XY}}$)	$d_{XY}(Ru) \rightarrow d^*_{X^2-Y^2}(Pt)$	98	3.45	359
T_{49} ($\mathbf{T_{CS\_XZ}}$)	$d_{XZ}(Ru) \rightarrow d^*_{X^2-Y^2}(Pt)$	99	3.45	359
T_{55} ($\mathbf{T_{Ru\_XZ\_X^2Y^2}}$)	$d_{XZ}(Ru) \rightarrow d^*_{X^2-Y^2}(Ru)$ $d_{XY}(Ru) \rightarrow d^*_{Z^2}(Ru)$	36 35	3.51	353
T_{56} ($\mathbf{T_{Ru\_XZ\_Z^2}}$)	$d_{XZ}(Ru) \rightarrow d^*_{Z^2}(Ru)$ $d_{XY}(Ru) \rightarrow d^*_{X^2-Y^2}(Ru)$	42 17	3.52	352
T_{60} ($\mathbf{T_{Ru\_XY\_Z^2}}$)	$d_{XZ}(Ru) \rightarrow d^*_{X^2-Y^2}(Ru)$ $d_{XY}(Ru) \rightarrow d^*_{Z^2}(Ru)$	42 35	3.58	346

[a] Weights larger than 10%.

Table S11 Vertical excitation energies (VEE), wavelengths (λ) and singly-excited configurations of the main triplet excited states calculated at the S_0 geometry for **$OsPtI_2$**.

State	Transition	Weight (%)	VEE (eV)	λ (nm)
T_1 ($\mathbf{T_{BL1\_YZ}}$)	$d_{YZ}(Os) \rightarrow \pi^*_{BL1}$ $d_{YZ}(Os) \rightarrow \pi^*_{BL4}$	58 26	1.96	633
T_2 (T_{Pt_YZ})	$d_{YZ}(Pt) \rightarrow d^*_{X^2-Y^2}(Pt)$ $d_{Z^2}(Pt) \rightarrow d^*_{X^2-Y^2}(Pt)$	62 20	2.11	586
T_3 ($\mathbf{T_{BL4\_XZ}}$)	$d_{XZ}(Os) \rightarrow \pi^*_{BL1}$ $d_{XZ}(Os) \rightarrow \pi^*_{BL4}$ $d_{XZ}(Os) \rightarrow \pi^*_{bpy1}$	34 28 20	2.12	585
T_4 ($\mathbf{T_{BL4\_YZ}}$)	$d_{YZ}(Os) \rightarrow \pi^*_{BL1}$ $d_{YZ}(Os) \rightarrow \pi^*_{BL4}$	33 31	2.12	585
T_5 ($T_{Pt\_Z^2}$)	$d_{Z^2}(Pt) \rightarrow d^*_{X^2-Y^2}(Pt)$ $d_{YZ}(Pt) \rightarrow d^*_{X^2-Y^2}(Pt)$ $d_{XY}(Pt) \rightarrow d^*_{X^2-Y^2}(Pt)$	61 19 13	2.14	580
T_6 ($\mathbf{T_{BL1\_XZ}}$)	$d_{XZ}(Os) \rightarrow \pi^*_{BL1}$ $d_{YZ}(Os) \rightarrow \pi^*_{BL2}$ $d_{XZ}(Os) \rightarrow \pi^*_{BL4}$ $d_{XZ}(Os) \rightarrow \pi^*_{bpy1}$	49 12 12 11	2.20	563
T_7 ($\mathbf{T_{BL1\_XY}}$)	$d_{XY}(Os) \rightarrow \pi^*_{BL1}$ $d_{YZ}(Os) \rightarrow \pi^*_{BL4}$ $d_{XY}(Os) \rightarrow \pi^*_{BL4}$	56 14 11	2.20	562
T_8 ($\mathbf{T_{bpy1\_YZ}}$)	$d_{YZ}(Os) \rightarrow \pi^*_{bpy1}$ $d_{XY}(Os) \rightarrow \pi^*_{BL1}$ $d_{YZ}(Os) \rightarrow \pi^*_{BL4}$	57 21 12	2.22	558
T_9 ($\mathbf{T_{bpy2\_YZ}}$)	$d_{YZ}(Os) \rightarrow \pi^*_{bpy2}$	85	2.24	553
T_{10} (T_{Pt_XZ})	$d_{XZ}(Pt) \rightarrow d^*_{X^2-Y^2}(Pt)$ $n_I[205] \rightarrow d^*_{X^2-Y^2}(Pt)$	85 11	2.30	538
T_{11} ($\mathbf{T_{bpy2\_XY}}$)	$d_{XY}(Os) \rightarrow \pi^*_{bpy2}$ $d_{XZ}(Os) \rightarrow \pi^*_{BL4}$	67 16	2.35	527
T_{12} ($\mathbf{T_{BL4\_XY}}$)	$d_{XY}(Os) \rightarrow \pi^*_{BL4}$ $d_{XZ}(Os) \rightarrow \pi^*_{BL2}$ $d_{XY}(Os) \rightarrow \pi^*_{BL1}$ $d_{XY}(Os) \rightarrow \pi^*_{bpy1}$	32 17 14 12	2.37	522
T_{13} (T_{BL2_YZ})	$d_{YZ}(Os) \rightarrow \pi^*_{BL2}$	71	2.38	520
T_{14} ($\mathbf{T_{bpy1\_XY}}$)	$d_{XY}(Os) \rightarrow \pi^*_{bpy1}$ $d_{XY}(Os) \rightarrow \pi^*_{BL4}$ $d_{XZ}(Os) \rightarrow \pi^*_{bpy2}$	47 31 16	2.39	519
T_{15} (T_{BL2_XZ})	$d_{XZ}(Os) \rightarrow \pi^*_{BL2}$ $d_{XY}(Os) \rightarrow \pi^*_{BL4}$ $d_{XY}(Os) \rightarrow \pi^*_{bpy1}$	46 15 11	2.48	499
T_{16} ($\mathbf{T_{bpy1\_XZ}}$)	$d_{XZ}(Os) \rightarrow \pi^*_{bpy1}$ $d_{XZ}(Os) \rightarrow \pi^*_{BL4}$ $d_{XY}(Os) \rightarrow \pi^*_{bpy2}$	47 22 17	2.53	490
T_{17} ($\mathbf{T_{bpy2\_XZ}}$)	$d_{XZ}(Os) \rightarrow \pi^*_{bpy2}$ $d_{XY}(Os) \rightarrow \pi^*_{bpy1}$ $d_{YZ}(Os) \rightarrow \pi^*_{BL1}$	50 15 10	2.58	479
T_{18}	$d_{YZ}(Pt) \rightarrow \pi^*_{BL1}$ $d_{XZ}(Os) \rightarrow \pi^*_{bpy2}$ $d_{YZ}(Pt) \rightarrow \pi^*_{BL3}$	27 22 22	2.59	478
T_{19} (T_{BL2_XY})	$d_{XY}(Os) \rightarrow \pi^*_{BL2}$	87	2.60	477
T_{20} (T_{Pt_XY})	$d_{XY}(Pt) \rightarrow d^*_{X^2-Y^2}(Pt)$ $d_{Z^2}(Pt) \rightarrow d^*_{X^2-Y^2}(Pt)$	73 15	2.64	469
T_{21} (T_{BL3_YZ})	$d_{YZ}(Os) \rightarrow \pi^*_{BL3}$	98	2.65	468
T_{22} (T_{MLCT})	$n_I \rightarrow d^*_{X^2-Y^2}(Pt)$ $d_{XZ}(Pt) \rightarrow \pi^*_{BL3}$ $d_{XZ}(Pt) \rightarrow \pi^*_{BL1}$	37 30 19	2.75	450
T_{23}	$d_{YZ}(Pt) \rightarrow \pi^*_{BL1}$ $\pi_{BL}[210] \rightarrow \pi^*_{BL1}$	53 11	2.76	448

T_{24}	$n_I \rightarrow d^*_{X^2-Y^2}(Pt)$ $d_{XZ}(Pt) \rightarrow \pi^*_{BL1}$ $d_{XZ}(Pt) \rightarrow \pi^*_{BL3}$	55 23 12	2.77	447
T_{25}	$d_{XZ}(Pt) \rightarrow \pi^*_{BL1}$ $d_{XZ}(Os) \rightarrow \pi^*_{BL3}$ $d_{XZ}(Pt) \rightarrow \pi^*_{BL3}$ $\pi_{BL} \rightarrow \pi^*_{BL1}$	34 29 13 10	2.81	441
T_{26}	$n_I \rightarrow \pi^*_{BL1}$	92	2.83	438
T_{27} (T_{BL3_XY})	$d_{XY}(Os) \rightarrow \pi^*_{BL3}$	97	2.85	435
T_{28}	$d_{YZ}(Pt) \rightarrow \pi^*_{BL3}$ $\pi_{BL}[210] \rightarrow \pi^*_{BL1}$	42 24	2.86	434
T_{29} (T_{BL3_XZ})	$d_{XZ}(Os) \rightarrow \pi^*_{BL3}$ $d_{XZ}(Pt) \rightarrow \pi^*_{BL3}$	59 23	2.86	433
T_{30}	$d_{Z^2}(Pt) \rightarrow \pi^*_{BL3}$ $d_{Z^2}(Pt) \rightarrow \pi^*_{BL1}$ $d_{XY}(Pt) \rightarrow \pi^*_{BL3}$	49 30 10	2.91	426
T_{31} (T_{IL})	$n_{BL} \rightarrow \pi^*_{BL1}$	88	2.99	415
T_{32} (T_{CS_YZ})	$d_{YZ}(Os) \rightarrow d^*_{X^2-Y^2}(Pt)$	99	3.03	409
T_{42} (T_{CS_XY})	$d_{XY}(Os) \rightarrow d^*_{X^2-Y^2}(Pt)$	98	3.23	384
T_{43} (T_{CS_XZ})	$d_{XZ}(Os) \rightarrow d^*_{X^2-Y^2}(Pt)$	97	3.23	383
T_{89} ($T_{Os\_YZ\_Z^2}$)	$d_{YZ}(Os) \rightarrow d^*_{Z^2}(Os)$ $d_{YZ}(Os) \rightarrow [249]$	52 23	3.96	312
T_{91} ($T_{Os\_YZ\_X^2Y^2}$)	$d_{YZ}(Os) \rightarrow d^*_{X^2-Y^2}(Os)$ $d_{YZ}(Os) \rightarrow \pi^*_{BL}[233]$ $d_{YZ}(Os) \rightarrow [248]$	39 27 13	3.98	311
T_{109} ($T_{Os\_XY\_X^2Y^2}$)	$d_{XY}(Os) \rightarrow d^*_{X^2-Y^2}(Os)$ $d_{XY}(Os) \rightarrow [248]$ $d_{XZ}(Os) \rightarrow d^*_{Z^2}(Os)$	50 16 15	4.26	290
T_{119} ($T_{Os\_XY\_Z^2}$)	$d_{XY}(Os) \rightarrow d^*_{Z^2}(Os)$ $d_{XY}(Os) \rightarrow [249]$ $d_{XZ}(Os) \rightarrow d^*_{X^2-Y^2}(Os)$	39 16 16	4.34	285
T_{124} ($T_{Os\_XZ\_Z^2}$)	$d_{XZ}(Os) \rightarrow d^*_{Z^2}(Os)$ $d_{XY}(Os) \rightarrow d^*_{X^2-Y^2}(Os)$ $d_{XZ}(Os) \rightarrow [249]$	34 16 14	4.36	284
T_{131} ($T_{Os\_XZ\_X^2Y^2}$)	$d_{XZ}(Os) \rightarrow d^*_{X^2-Y^2}(Os)$ $d_{XZ}(Os) \rightarrow [248]$ $d_{XY}(Os) \rightarrow d^*_{Z^2}(Os)$	52 16 13	4.41	281

[a] Weights larger than 10%.

Table S12 Vertical excitation energies (VEE), wavelengths (λ) and singly-excited configurations of the main triplet excited states calculated at the S_0 geometry for **Os**.

State	Transition	Weight (%)	VEE (eV)	λ (nm)
T_1 (**T_{BL4_YZ}**)	$d_{YZ}(Os) \rightarrow \pi^*_{BL4}$ $d_{YZ}(Os) \rightarrow \pi^*_{bpy1}$ $d_{YZ}(Os) \rightarrow \pi^*_{BL1}$	38 27 25	2.05	605
T_2 (**T_{BL4_XZ}**)	$d_{XZ}(Os) \rightarrow \pi^*_{bpy1}$ $d_{XZ}(Os) \rightarrow \pi^*_{BL4}$ $d_{XZ}(Os) \rightarrow \pi^*_{BL1}$	50 24 11	2.18	568
T_3 (**T_{bpy1_YZ}**)	$d_{YZ}(Os) \rightarrow \pi^*_{bpy1}$ $d_{YZ}(Os) \rightarrow \pi^*_{BL4}$	53 38	2.19	566
T_4 (**T_{bpy2_YZ}**)	$d_{YZ}(Os) \rightarrow \pi^*_{bpy2}$	87	2.21	562
T_5 (**T_{BL1_YZ}**)	$d_{YZ}(Os) \rightarrow \pi^*_{BL1}$ $d_{XY}(Os) \rightarrow \pi^*_{BL4}$	53 11	2.32	534
T_6 (**T_{bpy2_XY}**)	$d_{XY}(Os) \rightarrow \pi^*_{bpy2}$ $d_{XZ}(Os) \rightarrow \pi^*_{BL4}$	63 22	2.33	531
T_7 (**T_{BL4_XY}**)	$d_{XY}(Os) \rightarrow \pi^*_{BL4}$ $d_{XY}(Os) \rightarrow \pi^*_{BL1}$ $d_{YZ}(Os) \rightarrow \pi^*_{BL1}$	32 29 15	2.36	524
T_8 (**T_{bpy1_XY}**)	$d_{XY}(Os) \rightarrow \pi^*_{bpy1}$ $d_{XY}(Os) \rightarrow \pi^*_{BL4}$ $d_{XZ}(Os) \rightarrow \pi^*_{bpy2}$	45 24 22	2.37	522
T_9 (**T_{BL1_XZ}**)	$d_{XZ}(Os) \rightarrow \pi^*_{BL1}$ $d_{YZ}(Os) \rightarrow \pi^*_{BL2}$	63 17	2.43	510
T_{10} (**T_{bpy1_XZ}**)	$d_{XZ}(Os) \rightarrow \pi^*_{bpy1}$ $d_{XZ}(Os) \rightarrow \pi^*_{BL4}$ $d_{XY}(Os) \rightarrow \pi^*_{bpy2}$	39 27 21	2.50	495
T_{11} (**T_{BL2_XZ}**)	$d_{XY}(Os) \rightarrow \pi^*_{BL1}$ $d_{XZ}(Os) \rightarrow \pi^*_{BL2}$ $d_{XZ}(Os) \rightarrow \pi^*_{bpy2}$	27 26 13	2.54	488
T_{12} (**T_{BL2_YZ}**)	$d_{YZ}(Os) \rightarrow \pi^*_{BL2}$ $d_{XZ}(Os) \rightarrow \pi^*_{BL1}$ $d_{XZ}(Os) \rightarrow \pi^*_{BL4}$	70 10 10	2.57	482
T_{13} (**T_{bpy2_XZ}**)	$d_{XZ}(Os) \rightarrow \pi^*_{bpy2}$ $d_{XY}(Os) \rightarrow \pi^*_{bpy1}$	55 11	2.57	482
T_{14} (**T_{BL1_XY}**)	$d_{XY}(Os) \rightarrow \pi^*_{BL1}$ $d_{XY}(Os) \rightarrow \pi^*_{bpy1}$ $d_{XY}(Os) \rightarrow \pi^*_{BL4}$ $d_{XZ}(Os) \rightarrow \pi^*_{BL2}$	32 20 16 12	2.63	472
T_{15}	$\pi_{BL} \rightarrow \pi^*_{BL1}$ $d_{XZ}(Os) \rightarrow \pi^*_{BL2}$	38 34	2.79	445
T_{16} (**T_{BL2_XY}**)	$d_{XY}(Os) \rightarrow \pi^*_{BL2}$	91	2.80	442
T_{17}	$\pi_{BL}[200] \rightarrow \pi^*_{BL1}$	87	2.88	430
T_{18} (**T_{IL}**)	$n_{BL} \rightarrow \pi^*_{BL1}$	84	2.99	414
T_{19}	$\pi_{bpy}[198] \rightarrow \pi^*_{bpy2}$ $\pi_{bpy}[197] \rightarrow \pi^*_{BL4}$ $\pi_{bpy}[197] \rightarrow \pi^*_{bpy1}$	27 17 14	3.17	390
T_{20}	$\pi_{bpy}[197] \rightarrow \pi^*_{bpy2}$ $\pi_{bpy}[198] \rightarrow \pi^*_{BL4}$ $\pi_{bpy}[198] \rightarrow \pi^*_{bpy1}$	29 20 17	3.18	390
T_{21}	$\pi_{BL}[200] \rightarrow \pi^*_{BL2}$ $\pi_{BL} \rightarrow \pi^*_{BL1}$ $\pi_{BL}[195] \rightarrow \pi^*_{BL1}$	34 15 15	3.28	378
T_{22}	$\pi_{BL}[200] \rightarrow \pi^*_{BL2}$ $\pi_{BL}[195] \rightarrow \pi^*_{BL1}$ $d_{YZ}(Os) \rightarrow \pi^*_{bpy}[211]$ $\pi_{BL} \rightarrow \pi^*_{BL1}$	26 13 13 11	3.29	376
T_{23}	$d_{YZ}(Os) \rightarrow \pi^*_{bpy}[211]$	56	3.29	376
T_{24}	$d_{XY}(Os) \rightarrow \pi^*_{bpy}[211]$	48	3.35	369

	$d_{YZ}(Os) \rightarrow \pi^*_{bpy}[214]$	20		
T_{25}	$d_{YZ}(Os) \rightarrow \pi^*_{bpy}[213]$ $d_{XZ}(Os) \rightarrow \pi^*_{bpy}[211]$ $d_{YZ}(Os) \rightarrow \pi^*_{bpy}[215]$	41 17 12	3.37	368
T_{26}	$d_{YZ}(Os) \rightarrow \pi^*_{bpy}[215]$ $d_{XY}(Os) \rightarrow \pi^*_{bpy}[215]$	47 15	3.47	357
T_{27}	$\pi_{BL} \rightarrow \pi^*_{BL2}$ $\pi_{BL}[200] \rightarrow \pi^*_{BL4}$ $\pi_{BL}[200] \rightarrow \pi^*_{bpy1}$	39 26 12	3.50	354
T_{28}	$\sigma_{BL}[199] \rightarrow \pi^*_{BL1}$	87	3.55	349
T_{29}	$d_{XZ}(Os) \rightarrow \pi^*_{bpy}[211]$ $d_{YZ}(Os) \rightarrow \pi^*_{bpy}[213]$	49 33	3.55	349
T_{30}	$\pi_{BL} \rightarrow \pi^*_{BL3}$ $\pi_{BL} \rightarrow \pi^*_{BL4}$ $\pi_{BL}[195] \rightarrow \pi^*_{BL4}$	39 12 11	3.56	348
T_{34} ($\mathbf{T_{BL3\_YZ}}$)	$d_{YZ}(Os) \rightarrow \pi^*_{BL3}$	98	3.66	338
T_{41} ($\mathbf{T_{BL3\_XZ}}$)	$d_{XZ}(Os) \rightarrow \pi^*_{BL3}$ $\pi_{BL}[200] \rightarrow \pi^*_{BL3}$	63 19	3.80	326
T_{47} ($\mathbf{T_{BL3\_XY}}$)	$d_{XY}(Os) \rightarrow \pi^*_{BL3}$	98	3.88	319
T_{48} ($\mathbf{T_{Os\_YZ\_X^2Y^2}}$)	$d_{YZ}(Os) \rightarrow d^*_{X^2-Y^2}(Os)$ $d_{YZ}(Os) \rightarrow [227]$	64 24	3.95	314
T_{50} ($\mathbf{T_{Os\_YZ\_Z^2}}$)	$d_{YZ}(Os) \rightarrow d^*_{Z^2}(Os)$ $d_{YZ}(Os) \rightarrow [228]$ $\pi_{BL}[200] \rightarrow \pi^*_{BL3}$	36 14 11	3.96	313
T_{69} ($\mathbf{T_{Os\_XY\_X^2Y^2}}$)	$d_{XY}(Os) \rightarrow d^*_{X^2-Y^2}(Os)$ $d_{XZ}(Os) \rightarrow d^*_{Z^2}(Os)$ $d_{XY}(Os) \rightarrow [227]$	45 22 16	4.27	290
T_{75} ($\mathbf{T_{Os\_XY\_Z^2}}$)	$d_{XY}(Os) \rightarrow d^*_{Z^2}(Os)$ $d_{XZ}(Os) \rightarrow d^*_{X^2-Y^2}(Os)$ $d_{XY}(Os) \rightarrow [228]$	42 19 15	4.34	285
T_{77} ($\mathbf{T_{Os\_XZ\_Z^2}}$)	$d_{XZ}(Os) \rightarrow d^*_{Z^2}(Os)$ $d_{XY}(Os) \rightarrow d^*_{X^2-Y^2}(Os)$ $d_{XZ}(Os) \rightarrow [228]$ $d_{XY}(Os) \rightarrow \pi^*_{BL}[216]$	37 16 14 13	4.35	285
T_{85} ($\mathbf{T_{Os\_XZ\_X^2Y^2}}$)	$d_{XZ}(Os) \rightarrow d^*_{X^2-Y^2}(Os)$ $d_{XY}(Os) \rightarrow d^*_{Z^2}(Os)$ $\pi_{bpy}[197] \rightarrow \pi^*_{BL2}$ $d_{XZ}(Os) \rightarrow [227]$	32 14 11 11	4.42	280

[a] Weights larger than 10%.