

Supplementary Data

Synthesis of the ruthenium(II) bipyridyl *p*-bromobenzoyl-*N'*-(1,10-phenanthroline-5-yl)-thiourea [Ru(bpy)₂(phen-*p*-BrBT)](PF₆)₂

The reaction was performed under dark conditions and in inert argon gas. A 10% molar excess of *n*-benzoyl-*n'*-(1,10-phenanthroline-5-yl)thiourea (0.072 mmol) was dissolved in 10 mL of hot ethanol and was added to 0.064 mmol of *cis*-[Ru(bpy)₂Cl₂·2H₂O] dissolved in 5 mL of hot distilled water (H₂O). The mixture was heated for 3 hours at 100 °C. The solution was reduced to approximately one third of the original volume to give a precipitate. The solid was filtered off and then an excess amount of NH₄PF₆ (0.8 mmol) dissolved in cold distilled water was added into the filtrate, yielding a bright brown precipitate. The precipitate was then filtered through a Buchner funnel, washed with cold H₂O (3 x 10 mL), followed by cold diethyl ether (3 x 10 mL) and dried in vacuo.

Table I. TD-DFT calculated absorption bands and their composition for the [Ru(bpy)₂(phen-*p*-BrBT)]²⁺ complex. Transition with oscillator strength greater than 0.01 are shown, the major contributing transitions have more than 5% contribution to the absorption band.

Wavelength (nm)	Oscillator Strength	Transitions (characters) [contributions]
432.69	0.0345	HOMO-1 (Ru) → LUMO (π* _{bpy,phen}) [75%], HOMO-1(Ru) → LUMO+1 (π* _{bpy,phen}) [8%], HOMO (Ru) → LUMO+3 (π* _{bpy,phen}) [7%]
418.02	0.1450	HOMO-2 (Ru) → LUMO+2 (π* _{bpy,phen}) [28%], HOMO-1(Ru) → LUMO (π* _{bpy,phen}) [19%], HOMO-2 (Ru) → LUMO+1 (π* _{bpy,phen}) [12%], HOMO (Ru) → LUMO+3 (π* _{bpy,phen}) [10%], HOMO-1 (Ru) → LUMO+1 (π* _{bpy,phen}) [9%], HOMO-1 (Ru) → LUMO+2 (π* _{bpy,phen}) [7%], HOMO (Ru) → LUMO+2 (π* _{bpy,phen}) [5%]
414.66	0.1328	HOMO-2 (Ru) → LUMO+1 (π* _{bpy,phen}) (35%), HOMO-2 (Ru) → LUMO+2 (π* _{bpy,phen}) [16%], HOMO-1 (Ru) → LUMO+2 (π* _{bpy,phen}) [15%], HOMO-2 (Ru) → LUMO (π* _{bpy,phen}) [12%], HOMO-1 (Ru) → LUMO+3 (π* _{bpy,phen}) [10%], HOMO-1 (Ru) → LUMO+1 (π* _{bpy,phen}) [7%]
398.31	0.0419	HOMO-2 (Ru) → LUMO+3 (π* _{bpy,phen}) [71%], HOMO-1 (Ru) → LUMO+3 (π* _{bpy,phen}) [8%], HOMO-2 (Ru) → LUMO+2 (π* _{bpy,phen}) [7%]
397.06	0.0267	HOMO-1 (Ru) → LUMO+3 (π* _{bpy,phen}) [56%], HOMO-1 (Ru) → LUMO+1 (π* _{bpy,phen}) [15%], HOMO-2 (Ru) → LUMO+3 (π* _{bpy,phen}) [12%], HOMO-1 (Ru) → LUMO+2 (π* _{bpy,phen}) [12%]
328.49	0.0164	HOMO-2 (Ru) → LUMO+5 (π* _{bpy}) [93%]
315.99	0.0258	HOMO (Ru) → LUMO+8 (π* _{bpy}) [85%], HOMO-1 (Ru) → LUMO+6 (π* _{bpy}) [7%]
311.34	0.0340	HOMO-1 (Ru) → LUMO+6 (π* _{bpy}) [83%], HOMO (Ru) → LUMO+8 (π* _{bpy}) [7%]
307.91	0.0166	HOMO-1 (Ru) → LUMO+7 (π* _{bpy}) [82%]
304.19	0.1551	HOMO-4 (<i>n</i> _{C-S}) → LUMO+4 (π* _{BrBT}) [85%]
303.66	0.0408	HOMO-2 (Ru) → LUMO+8 (π*) [74%], HOMO-4 (<i>n</i> _{C-S}) → LUMO+4 (π* _{BrBT}) [6%], HOMO-7 (π _{bpy}) → LUMO (π* _{bpy,phen}) [5%]
297.55	0.0627	HOMO-1 (Ru) → LUMO+8 (π* _{bpy}) [28%], HOMO-2 (Ru) → LUMO+6 (π* _{bpy}) [16%], HOMO-2 (Ru) → LUMO+7 (π* _{bpy}) [14%], HOMO-6 (Ru) → LUMO (π* _{bpy}) [11%], HOMO (Ru) → LUMO+7 (π* _{bpy}) [8%], HOMO-1 (Ru) → LUMO +9 (π* _{phen}) [8%]
293.40	0.0364	HOMO-7 (π _{bpy}) → LUMO (π* _{bpy,phen}) [16%], HOMO-9 (π _{phen}) → LUMO (π* _{bpy,phen}) [11%], HOMO-8 (π _{phen}) → LUMO+3 (π* _{bpy,phen}) [10%], HOMO-6 (π _{bpy}) → LUMO+1 (π* _{bpy,phen}) [7%], HOMO-8 (π _{phen}) → LUMO +2 (π* _{bpy,phen}) [7%], HOMO-5 (BrBz) → LUMO (π* _{bpy,phen}) [6%], HOMO-5 (π* _{BrBT}) → LUMO+1 (π*) [6%], HOMO-6 (π _{bpy}) → LUMO +3 (π* _{bpy,phen}) [5%]
292.99	0.0157	HOMO-6 (π _{bpy}) → LUMO (π* _{bpy,phen}) [55%], HOMO-8 (π _{phen}) → LUMO (π* _{bpy,phen}) [19%]
284.93	0.0268	HOMO-5 (π _{BrBT}) → LUMO+1 (π* _{bpy,phen}) [34%], HOMO-5 (π* _{BrBT}) → LUMO +3 (π*

281.22	0.0902	$\pi_{\text{bpy,phen}}^*$ [20%], HOMO-5 (π_{BrBT}) \rightarrow LUMO+2 ($\pi_{\text{bpy,phen}}^*$) [17%], HOMO-6 (π_{bpy}) \rightarrow LUMO+3 ($\pi_{\text{bpy,phen}}^*$) [6%] HOMO-5 (π_{BrBT}) \rightarrow LUMO ($\pi_{\text{bpy,phen}}^*$) [5%] HOMO-7 (π_{bpy}) \rightarrow LUMO+1 ($\pi_{\text{bpy,phen}}^*$) [23%], HOMO-7 (π_{bpy}) \rightarrow LUMO+2 ($\pi_{\text{bpy,phen}}^*$) [20%], HOMO-7 (π_{bpy}) \rightarrow LUMO+3 ($\pi_{\text{bpy,phen}}^*$) [16%], HOMO-8 (π_{phen}) \rightarrow LUMO+3 ($\pi_{\text{bpy,phen}}^*$) [7%]
280.97	0.0771	HOMO-8 (π_{phen}) \rightarrow LUMO+2 ($\pi_{\text{bpy,phen}}^*$) [22%], HOMO-5 (π_{BrBT}) \rightarrow LUMO+2 ($\pi_{\text{bpy,phen}}^*$) [15%], HOMO-5 (π_{BrBT}) \rightarrow LUMO+3 ($\pi_{\text{bpy,phen}}^*$) [15%], HOMO-8 (π_{phen}) \rightarrow LUMO+3 ($\pi_{\text{bpy,phen}}^*$) [14%], HOMO-5 (π_{BrBT}) \rightarrow LUMO+2 ($\pi_{\text{bpy,phen}}^*$) [6%], HOMO-5 (π_{BrBT}) \rightarrow LUMO+3 ($\pi_{\text{bpy,phen}}^*$) [5%]
280.08	0.0554	HOMO-5 (π_{BrBT}) \rightarrow LUMO+1 ($\pi_{\text{bpy,phen}}^*$) [30%], HOMO-5 (π_{BrBT}) \rightarrow LUMO+2 ($\pi_{\text{bpy,phen}}^*$) [18%], HOMO-8 (π_{phen}) \rightarrow LUMO +1 ($\pi_{\text{bpy,phen}}^*$) [12%], HOMO-7 (π_{bpy}) \rightarrow LUMO+3 ($\pi_{\text{bpy,phen}}^*$) [10%], HOMO-5 (π_{BrBT}) \rightarrow LUMO ($\pi_{\text{bpy,phen}}^*$) [5%]
278.94	0.3612	HOMO-7 (π_{bpy}) \rightarrow LUMO +3 ($\pi_{\text{bpy,phen}}^*$) [40%], HOMO-5 (π_{BrBT}) \rightarrow LUMO+4 (π_{BrBT}^*) [10%], HOMO-8 (π_{phen}) \rightarrow LUMO+1 ($\pi_{\text{bpy,phen}}^*$) [7%], HOMO-2 (Ru) \rightarrow LUMO+7 (π_{bpy}^*) [7%], HOMO-7 (π_{bpy}) \rightarrow LUMO +2 (π^*) [5%]
278.58	0.0923	HOMO-5 (π_{BrBT}) \rightarrow LUMO+4 (π_{BrBT}^*) [46%], HOMO-8 (π_{phen}) \rightarrow LUMO+4 (π_{BrBT}^*) [9%], HOMO-12 (π_{BrBT}) \rightarrow LUMO+4 (π_{BrBT}^*) [6%], HOMO-7 (π_{bpy}) \rightarrow LUMO+3 ($\pi_{\text{bpy,phen}}^*$) [5%], HOMO-7 (π_{bpy}) \rightarrow LUMO+3 ($\pi_{\text{bpy,phen}}^*$) [5%]
277.42	0.2220	HOMO-5 (π_{BrBT}) \rightarrow LUMO+3 ($\pi_{\text{bpy,phen}}^*$) [31%], HOMO-5 (π_{BrBT}) \rightarrow LUMO+2 ($\pi_{\text{bpy,phen}}^*$) [20%], HOMO-6 (π_{bpy}) \rightarrow LUMO+3 ($\pi_{\text{bpy,phen}}^*$) [10%], HOMO-7 (π_{bpy}) \rightarrow LUMO+1 ($\pi_{\text{bpy,phen}}^*$) [7%], HOMO-6 (π_{bpy}) \rightarrow LUMO+2 ($\pi_{\text{bpy,phen}}^*$) [7%]
276.09	0.3505	HOMO-8 (π_{phen}) \rightarrow LUMO+3 ($\pi_{\text{bpy,phen}}^*$) [28%], HOMO-8 (π_{phen}) \rightarrow LUMO+2 ($\pi_{\text{bpy,phen}}^*$) [16%], HOMO-5 (π_{BrBT}) \rightarrow LUMO+3 ($\pi_{\text{bpy,phen}}^*$) [10%], HOMO-5 (π_{BrBT}) \rightarrow LUMO+2 ($\pi_{\text{bpy,phen}}^*$) [7%], HOMO-7 (π_{phen}) \rightarrow LUMO+1 ($\pi_{\text{bpy,phen}}^*$) [7%], HOMO-2 (Ru) \rightarrow LUMO+8 (π_{bpy}^*) [6%]
271.52	0.2461	HOMO-8 (π_{phen}) \rightarrow LUMO+4 (π_{BrBT}^*) [28%], HOMO-5 (π_{BrBT}) \rightarrow LUMO+4 (π_{BrBT}^*) [18%], HOMO-9 (π_{phen}) \rightarrow LUMO+1 ($\pi_{\text{bpy,phen}}^*$) [13%], HOMO-6 (π_{bpy}) \rightarrow LUMO +4 (π_{BrBT}^*) [10%], HOMO-12 (π_{BrBT}) \rightarrow LUMO+4 (π_{BrBT}^*) [8%], HOMO-9 (π_{phen}) \rightarrow LUMO ($\pi_{\text{bpy,phen}}^*$) [7%], HOMO-3 (Ru) \rightarrow LUMO+11 (π_{BrBT}^*) [5%]
271.30	0.0711	HOMO-9 (π_{phen}) \rightarrow LUMO ($\pi_{\text{bpy,phen}}^*$) [33%], HOMO-9 (π_{phen}) \rightarrow LUMO+1 ($\pi_{\text{bpy,phen}}^*$) [32%], HOMO-9 (π_{phen}) \rightarrow LUMO+2 ($\pi_{\text{bpy,phen}}^*$) [11%], HOMO-5 (π_{BrBT}) \rightarrow LUMO+4 (π_{BrBT}^*) [6%], HOMO-8 (π_{phen}) \rightarrow LUMO+4 (π_{BrBT}^*) [5%]
266.64	0.0179	HOMO-9 (π_{phen}) \rightarrow LUMO+3 ($\pi_{\text{bpy,phen}}^*$) [47%], HOMO-3 (Ru) \rightarrow LUMO+9 (π_{phen}^*) [17%], HOMO-3 (Ru) \rightarrow LUMO+8 (π_{bpy}^*) [6%], HOMO-4 ($n_{\text{C-S}}$) \rightarrow LUMO+5 (π_{bpy}^*) [6%]
265.18	0.0297	HOMO-3 (Ru) \rightarrow LUMO+11 (π_{BrBT}^*) (38%), HOMO-3 (Ru) \rightarrow LUMO+10 (π_{BrBT}^*) (29%), HOMO-9 (π_{phen}) \rightarrow LUMO+3 ($\pi_{\text{bpy,phen}}^*$) [7%], HOMO-8 (π_{phen}) \rightarrow LUMO +4 (π_{BrBT}^*) [6%]
261.80	0.0315	HOMO-3 (Ru) \rightarrow LUMO+8 (π_{bpy}^*) [52%], HOMO-3 (Ru) \rightarrow LUMO+9 (π_{phen}^*) [18 %], HOMO-9 (π_{phen}) \rightarrow LUMO+3 ($\pi_{\text{bpy,phen}}^*$) [8%]
259.19	0.6078	HOMO-9 (π_{phen}) \rightarrow LUMO ($\pi_{\text{bpy,phen}}^*$) [24%], HOMO-9 (π_{phen}) \rightarrow LUMO+1 ($\pi_{\text{bpy,phen}}^*$) [17%], HOMO-9 (π_{phen}) \rightarrow LUMO+2 ($\pi_{\text{bpy,phen}}^*$) [11%], HOMO-8 (π_{phen}) \rightarrow LUMO+3 ($\pi_{\text{bpy,phen}}^*$) [11%]
250.26	0.0607	HOMO-1 (Ru) \rightarrow LUMO+12 (π_{phen}^*) [45%], HOMO-1 (Ru) \rightarrow LUMO+10 (π_{BrBT}^*) [29%], HOMO-1 (Ru) \rightarrow LUMO+11 (π_{BrBT}^*) [13%]
245.81	0.0500	HOMO-7 (π_{phen}) \rightarrow LUMO+5 (π_{bpy}^*) [54%]
241.27	0.0571	HOMO-5 (π_{BrBT}) \rightarrow LUMO +5 (π_{bpy}^*) [46%], HOMO-8 (π_{phen}) \rightarrow LUMO+5 (π_{bpy}^*) [31%]

Table II. TD-DFT calculated absorption bands and their composition for the [Ru(phen)₂(phen-*p*-BrBT)]²⁺ complex. Transition with oscillator strength greater than 0.01 are shown, the major contributing transitions have more than 5% contribution to the absorption band.

Wavelength (nm)	Oscillator Strength	Transitions (characters) [contributions]
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431.38	0.0504	HOMO-1 (Ru) → LUMO (π^*_{phen}) [45%] HOMO-1(Ru) → LUMO+1 (π^*_{phen}) [10%], HOMO (Ru) → LUMO (π^*_{phen}) [6%], HOMO(Ru) → LUMO+1 (π^*_{phen}) [26%], HOMO(Ru) → LUMO+2 (π^*_{phen}) [5%]
424.70	0.0297	HOMO-1 (Ru) → LUMO+2 (π^*_{phen}) [27%], HOMO (Ru) → LUMO+1 (π^*_{phen}) [23%], HOMO-2 (Ru) → LUMO (π^*_{phen}) [15%], HOMO-2 (Ru) → LUMO+1 (π^*_{phen}) [13%], HOMO (Ru) → LUMO (π^*_{phen}) [5%],
418.77	0.0998	HOMO-1 (Ru) → LUMO+3 (π^*_{bpy}) [38%], HOMO-1 (Ru) → LUMO (π^*_{phen}) [13%]. HOMO-2 (Ru) → LUMO+1 (π^*_{phen}) [7%]
413.71	0.1076	HOMO-1 → LUMO+3 (π^*_{phen}) [40%], HOMO-2 (Ru) → LUMO+2 (π^*_{phen}) [34%], HOMO-2 (Ru) → LUMO+1 (π^*_{phen}) [12%], HOMO (Ru) → LUMO+5 (π^*_{phen}) [7%]
405.53	0.0641	HOMO-2 → LUMO+1 (π^*_{phen}) [22%], HOMO-1 (Ru) → LUMO (π^*_{phen}) [16%], HOMO-1 (Ru) → LUMO (π^*_{phen}) → LUMO+1 (π^*_{phen}) [20%], HOMO (Ru) → LUMO (π^*_{phen}) [21%], HOMO-2 (Ru) → LUMO (π^*_{phen}) [5%]
401.77	0.0628	HOMO-1 (Ru) → LUMO+1 (π^*_{phen}) [37%], HOMO-1 (Ru) → LUMO+2 (π^*_{phen}) [13%], HOMO (Ru) → LUMO+4 (π^*_{phen}) [17%], HOMO-2 (Ru) → LUMO +1 (π^*_{phen}) [6%]
395.87	0.0671	HOMO (Ru) → LUMO+5 (π^*_{phen}) [81%]
383.90	0.0410	HOMO-1 (Ru) → LUMO +4 (π^*_{phen}) [76%]
376.23	0.0350	HOMO-2 (Ru) → LUMO +5 (π^*_{phen}) [89%]
357.67	0.0272	HOMO-4 (π_{BrBT}) → LUMO (π^*_{phen}) [55%], HOMO-4 (π_{BrBT}) → LUMO+1 (π^*_{phen}) [18%], HOMO-4 ($n_{\text{C=S}}$) → LUMO (π^*_{BrBT}) [15%]
342.43	0.0256	HOMO-4 (π_{BrBT}) → LUMO+1 (π^*_{phen}) [54%], HOMO-4 (π_{BrBT}) → LUMO+2 (π^*_{phen}) [18%], HOMO-4 (π_{BrBT}) → LUMO (π^*_{phen}) [6%],
310.11	0.0602	HOMO-4 (π_{BrBT}) → LUMO+6 (π^*_{BrBT}) [75%], HOMO-4 (π_{BrBT}) → LUMO+4 (π^*_{phen}) [7%], HOMO-3 ($n_{\text{C=S}}$) → LUMO+4 (π^*_{phen}) [7%]
302.58	0.0347	HOMO-4 (π_{BrBT}) → LUMO+4 (π^*_{phen}) [71%], HOMO-8 (π_{phen} & $n_{\text{C=S}}$) → LUMO (π^*_{phen}) [7%], HOMO-5 (π_{phen}) → LUMO (π^*_{phen}) [9%]
302.50	0.0885	HOMO-5 (π_{phen}) → LUMO (π^*_{phen}) [30%], HOMO-4 (π_{BrBT}) → LUMO+5 (π^*_{phen}) [23%], HOMO-8 (π_{phen} & $n_{\text{C=S}}$) → LUMO (π^*_{phen}) [7%],
301.14	0.1446	HOMO-8 (π_{phen} & $n_{\text{C=S}}$) → LUMO + 1(π^*_{phen}) [9%], HOMO-7 (π_{phen}) → LUMO (π^*_{phen}) [30%], HOMO-5 (π_{phen}) → LUMO+1 (π^*_{phen}) [13%], HOMO-1 (Ru) → LUMO +7 (π^*_{phen}) [10%]
300.34	0.0764	HOMO-7 (π_{phen}) → LUMO (π^*_{phen}) [8%], HOMO-6 (π_{phen}) → LUMO (π^*_{phen}) [48%], HOMO-6 (π_{phen}) → LUMO+2 (π^*_{phen}) [10%], HOMO-5 (π_{phen}) → LUMO+1 (π^*_{phen}) [6%]
299.29	0.0872	HOMO-7 (π_{phen}) → LUMO (π^*_{phen}) [23%], HOMO-7 (π_{phen}) → LUMO+2 (π^*_{phen}) [8%], HOMO-6 (π_{phen}) → LUMO (π^*_{phen}) [15%], HOMO-6 (π_{phen}) → LUMO+2 (π^*_{phen}) [9%], HOMO-5 (π_{phen}) → LUMO+1 (π^*_{phen}) [6%]
286.81	0.0742	HOMO-8 (π_{phen} & $n_{\text{C=S}}$) → LUMO + 1(π^*_{phen}) [7%], HOMO-8 (π_{phen} & $n_{\text{C=S}}$) → LUMO + 2(π^*_{phen}) [8%], HOMO-5 (π_{phen}) → LUMO (π^*_{phen}) [9%], HOMO-5 (π_{phen}) → LUMO+1 (π^*_{phen}) [32%], HOMO (Ru) → LUMO+9 (π^*_{phen}) [5%]
278.45	0.0352	HOMO-3 ($n_{\text{C=S}}$) → LUMO +7 (π^*_{phen}) [25%], HOMO-8 (π_{phen} & $n_{\text{C=S}}$) → LUMO + 1(π^*_{phen}) [9%], HOMO-1 (Ru) → LUMO +8 (π^*_{ligands}) [19%]
276.47	0.4559	HOMO-5 (π_{phen}) → LUMO ($\pi^*_{\text{phen-BrBT}}$) [42%], HOMO-8 (π^*_{phen} & $n_{\text{C=S}}$) → LUMO + 6($\pi^*_{\text{phen-BrBT}}$) [16%]
272.95	0.0772	HOMO-10 (π_{phen}) → LUMO+1 (π^*_{phen}) [9%], HOMO-10 (π_{phen}) → LUMO+3 (π^*_{phen}) [22%], HOMO-9 (π_{phen}) → LUMO+2 (π^*_{phen}) [26%]
271.87	0.0249	HOMO-10 (π_{phen}) → LUMO+1 (π^*_{phen}) [15%], HOMO-10 (π_{phen}) → LUMO+2 (π^*_{phen}) [7%], HOMO-9 (π_{phen}) → LUMO+2 (π^*_{phen}) [12%], HOMO-8 ($\pi^*_{\text{phen-BT}}$) → LUMO+3 (π^*_{phen}) [15%], HOMO-5 (π_{phen}) → LUMO+4 (π^*_{phen}) [8%]
270.66	0.0248	HOMO-11 (π_{phen}) → LUMO+1 (π^*_{phen}) [11%], HOMO-10 (π_{phen}) → LUMO+1 (π^*_{phen}) [14%], HOMO-9 (π_{phen}) → LUMO+3 (π^*_{phen}) [7%], HOMO-10 (π_{phen}) → LUMO+3 (π^*_{phen}) [16%], HOMO-5 (π_{phen}) → LUMO+4 (π^*_{phen}) [23%]
269.49	0.0227	HOMO-11 (π_{phen}) → LUMO (π^*_{phen}) [13%], HOMO-11 (π_{phen}) → LUMO+1 (π^*_{phen}) [7%], HOMO-10 (π_{phen}) → LUMO+2 (π^*_{phen}) [32%]
266.16	0.0195	HOMO-11 (π_{phen}) → LUMO+3 (π^*_{phen}) [74%]
265.92	0.0628	HOMO-9 (π_{phen}) → LUMO+4 (π^*_{phen}) [28%], HOMO-10 ($\pi_{\text{phen-BrBT}}$) → LUMO+4 (π^*_{phen}) [30%], HOMO-5 (π_{phen}) → LUMO+4 (π^*_{phen}) [11%]
263.84	0.0762	HOMO-9 (π_{phen}) → LUMO+5 (π^*_{phen}) [23%], HOMO-8 ($\pi_{\text{phen-BrBT}}$) → LUMO+5 (π^*_{phen}) [20%], HOMO-5 (π_{phen}) → LUMO+5 (π^*_{phen}) [8%]

263.65	0.1416	HOMO-11 (π_{phen}) \rightarrow LUMO (π^*_{phen}) [8%], HOMO-9 (π_{phen}) \rightarrow LUMO+4 (π^*_{phen}) [18%], HOMO-8 ($\pi_{\text{phen-BrBT}}$) \rightarrow LUMO+4 (π^*_{phen}) [16%], HOMO-11 (π_{phen}) \rightarrow LUMO+2 (π^*_{phen}) [9%]
260.93	0.0217	HOMO-6 (π_{phen}) \rightarrow LUMO+6 (π^*_{phen}) [34%], HOMO-7 (π_{phen}) \rightarrow LUMO+6 (π^*_{phen}) [8%], HOMO-10 (π_{phen}) \rightarrow LUMO+4 (π^*_{phen}) [7%], HOMO-8 ($\pi_{\text{phen-BrBT}}$) \rightarrow LUMO+5 (π^*_{phen}) [6%], HOMO-9 (π_{phen}) \rightarrow LUMO+5 (π^*_{phen}) [5%]
260.33	0.2027	HOMO-6 (π_{phen}) \rightarrow LUMO+6 ($\pi^*_{\text{phen-BrBT}}$) [28%], HOMO-11 (π_{phen}) \rightarrow LUMO+2 (π^*_{phen}) [13%]
260.02	0.0232	HOMO-9 (π_{phen}) \rightarrow LUMO+5 (π^*_{phen}) [34%], HOMO-10 (π_{phen}) \rightarrow LUMO+5 (π^*_{phen}) [21%], HOMO-10 ($\pi_{\text{phen-BrBT}}$) \rightarrow LUMO+5 (π^*_{phen}) [18%]
259.72	0.0745	HOMO-7 (π_{phen}) \rightarrow LUMO+6 ($\pi^*_{\text{phen-BrBT}}$) [17%], HOMO-10 (π_{phen}) \rightarrow LUMO+3 (π^*_{phen}) [14%], HOMO-6 (π_{phen}) \rightarrow LUMO+5 (π^*_{phen}) [10%], HOMO-8 ($\pi_{\text{phen-BrBT}}$) \rightarrow LUMO+5 (π^*_{phen}) [6%], HOMO-9 (π_{phen}) \rightarrow LUMO+2 (π^*_{phen}) [5%]
259.48	0.0439	HOMO-7 (π_{phen}) \rightarrow LUMO+6 ($\pi^*_{\text{phen-BrBT}}$) [46%], HOMO (Ru) \rightarrow LUMO+11 ($\pi^*_{\text{phen-BrBT}}$) [10%], HOMO-6 (π_{phen}) \rightarrow LUMO+6 ($\pi^*_{\text{phen-BrBT}}$) [7%], HOMO (Ru) \rightarrow LUMO+10 (π^*_{Bz}) [7%]
258.78	0.0535	HOMO (Ru) \rightarrow LUMO+10 (π^*_{Bz}) [21%], HOMO-7 (π_{phen}) \rightarrow LUMO+6 ($\pi^*_{\text{phen-BrBT}}$) [13%], HOMO-4 (π_{BrBT}) \rightarrow LUMO+7 (π^*_{phen}) [8%]
258.36	0.0340	HOMO-12 (π^*_{Bz}) \rightarrow LUMO (π^*_{phen}) [42%], HOMO-12 (π_{Bz}) \rightarrow LUMO+1 (π^*_{phen}) [13%], HOMO-4 (π_{BrBT}) \rightarrow LUMO+7 (π^*_{phen}) [13%]
257.76	0.1299	HOMO-11 (π_{phen}) \rightarrow LUMO+4 (π^*_{phen}) [29%], HOMO-4 (π_{BrBT}) \rightarrow LUMO+7 (π^*_{phen}) [17%], HOMO-12 (π_{Bz}) \rightarrow LUMO (π^*_{phen}) [14%]
256.86	0.0637	HOMO-11 (π_{phen}) \rightarrow LUMO+4 (π^*_{phen}) [57%], HOMO-4 (π_{BrBT}) \rightarrow LUMO+7 (π^*_{phen}) [19%]
256.59	0.8369	HOMO-9 (π_{phen}) \rightarrow LUMO+3 (π^*_{phen}) [18%], HOMO-10 (π_{phen}) \rightarrow LUMO+2 (π^*_{phen}) [12%], HOMO-6 (π_{phen}) \rightarrow LUMO+4 (π^*_{phen}) [10%], HOMO-7 (π_{phen}) \rightarrow LUMO+5 (π^*_{phen}) [7%]
255.92	0.0516	HOMO-8 ($\pi_{\text{phen-BrBT}}$) \rightarrow LUMO+6 ($\pi^*_{\text{phen-BrBT}}$) [29%], HOMO-14 (π_{BrBT}) \rightarrow LUMO+7 ($\pi^*_{\text{phen-BrBT}}$) [15%], HOMO-14 (π_{BrBT}) \rightarrow LUMO+1 (π^*_{phen}) [13%], HOMO-14 (π_{BrBT}) \rightarrow LUMO (π^*_{phen}) [10%], HOMO-4 (π_{BrBT}) \rightarrow LUMO+5 ($\pi^*_{\text{phen-BrBT}}$) [7%]
253.84	0.1092	HOMO-1 (Ru) \rightarrow LUMO+11 ($\pi^*_{\text{phen-BrBT}}$) [18%], HOMO-1 (Ru) \rightarrow LUMO+10 (π^*_{phen}) [14%], HOMO-2 (Ru) \rightarrow LUMO+11 ($\pi^*_{\text{phen-BrBT}}$) [9%], HOMO-2 (Ru) \rightarrow LUMO+10 (π^*_{Bz}) [7%]
252.97	0.0870	HOMO-2 (Ru) \rightarrow LUMO+11 (π^*_{phen}) [28%], HOMO-2 (Ru) \rightarrow LUMO+10 (π^*_{phen}) [24%], HOMO-1 (Ru) \rightarrow LUMO+11 (π^*_{phen}) [5%]
250.99	0.0220	HOMO-12 (π_{Bz}) \rightarrow LUMO+10 (π^*_{phen}) [53%], HOMO-12 (π_{Bz}) \rightarrow LUMO+11 (π^*_{phen}) [28%]
247.92	0.0424	HOMO (Ru) \rightarrow LUMO+15 (π^*_{phen}) [73%], HOMO (Ru) \rightarrow LUMO+14 (π^*_{phen}) [15%]
247.55	0.0516	HOMO-11 (π_{phen}) \rightarrow LUMO+6 ($\pi^*_{\text{phen-BrBT}}$) [48%], HOMO-12 (π_{Bz}) \rightarrow LUMO+6 ($\pi^*_{\text{phen-BrBT}}$) [7%], HOMO-12 (π_{Bz}) \rightarrow LUMO+6 ($\pi^*_{\text{phen-BrBT}}$) [7%]
244.26	0.0313	HOMO-1 (Ru) \rightarrow LUMO+13 (π^*_{ligand}) [39%], HOMO-2 (Ru) \rightarrow LUMO+15 ($\pi^*_{\text{phen-BrBT}}$) [37%], HOMO (Ru) \rightarrow LUMO+14 (π^*_{phen}) [12%]