Supporting Information

Molecular engineering for optical properties of 5-substituted-1,10-phenanthroline-based Ru(II) complexes

Elodie ROUSSET
Olivier MONGIN
Juliette MOREAU
Latévi Max LAWSON-DAKU
Marc BELEY
Philippe GROS
Sylviane CHEVREUX
Mireille BLANCHARD-DESCE
Gilles LEMERCIER

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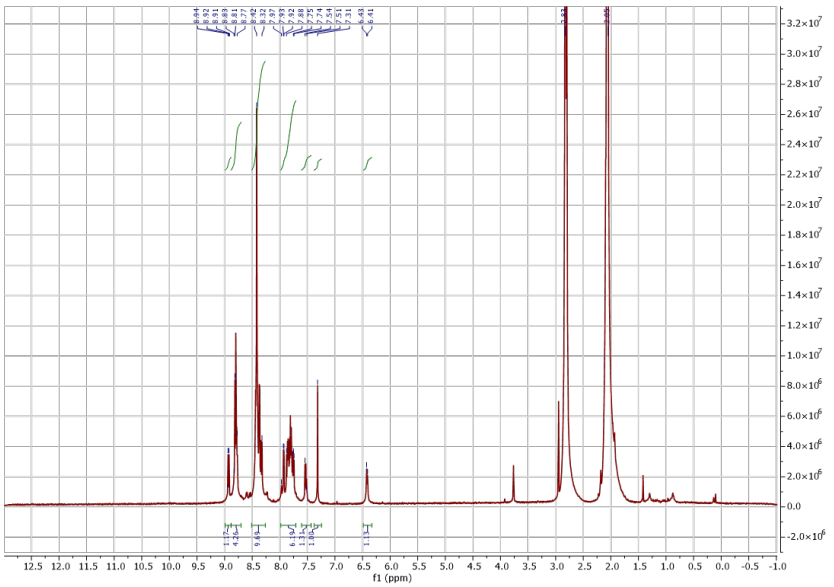
S1 ^{1}H NMR spectra of Ru(II) complexes recorded at 250.1 MHz



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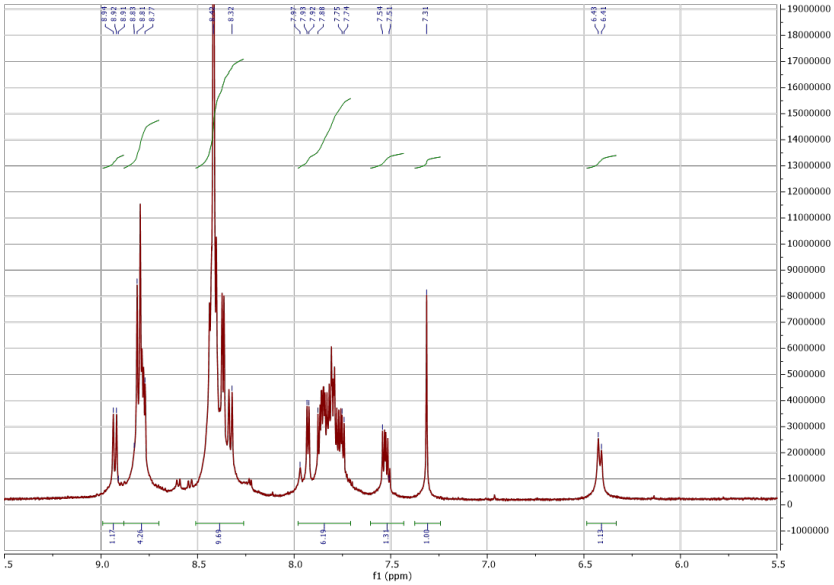
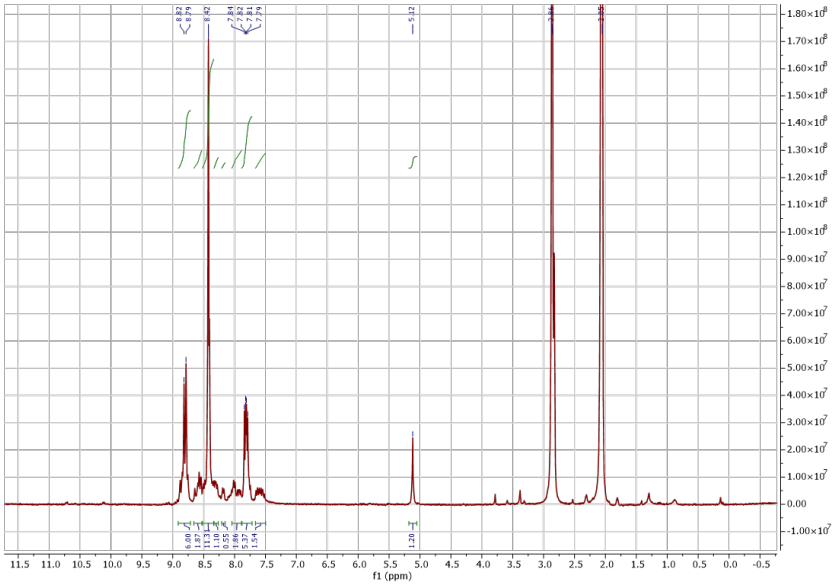


Figure S1: ^{1}H NMR spectrum of $[Ru(phen)_2(phen\text{-}NH_2)](PF6)_2$ in CD_3CO.



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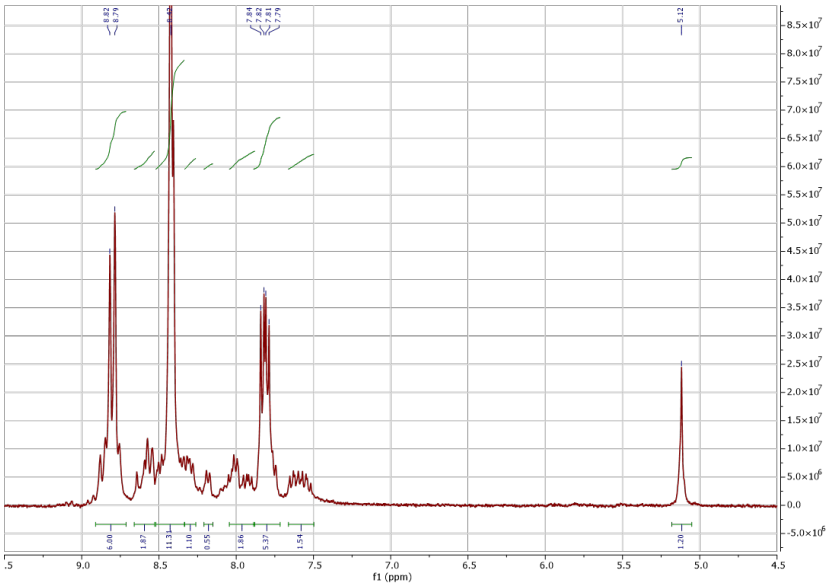
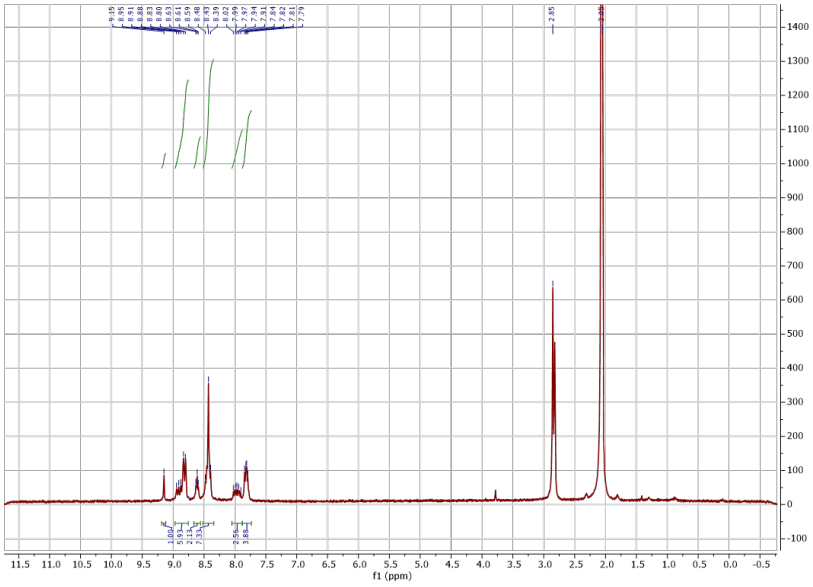


Figure S2: ^{1}H NMR spectrum of [Ru(phen)$_2$(phen-epox)](PF6)$_2$ in CD_3CO.



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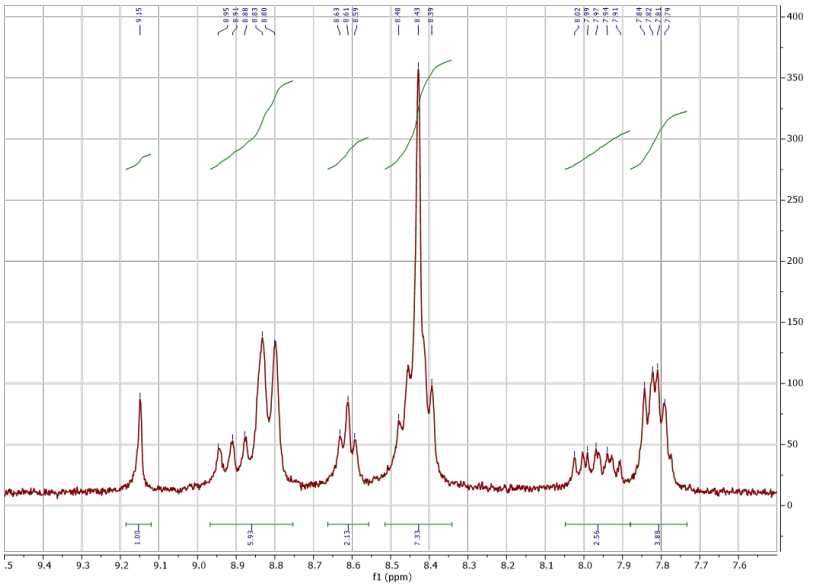
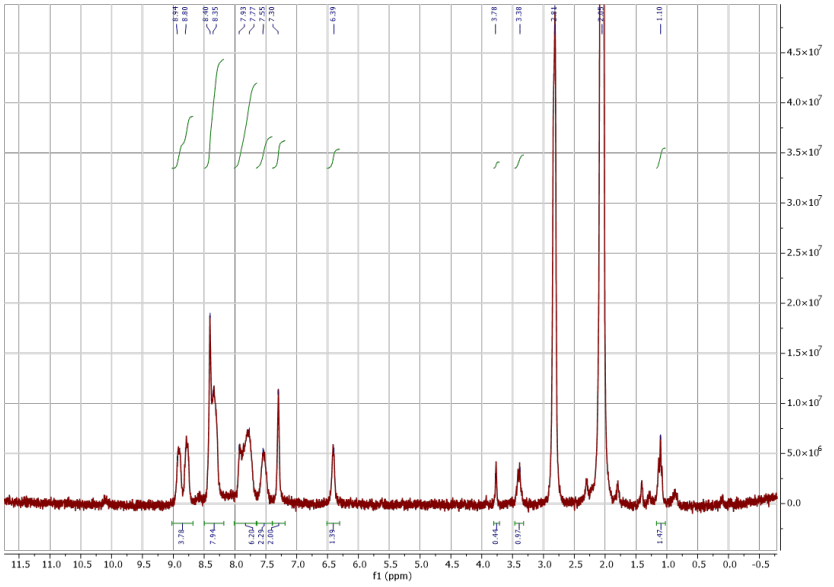


Figure S3: ^{1}H NMR spectrum of [Ru(phen)$_2$(phen-CN)](PF6)$_2$ in CD_3CO.



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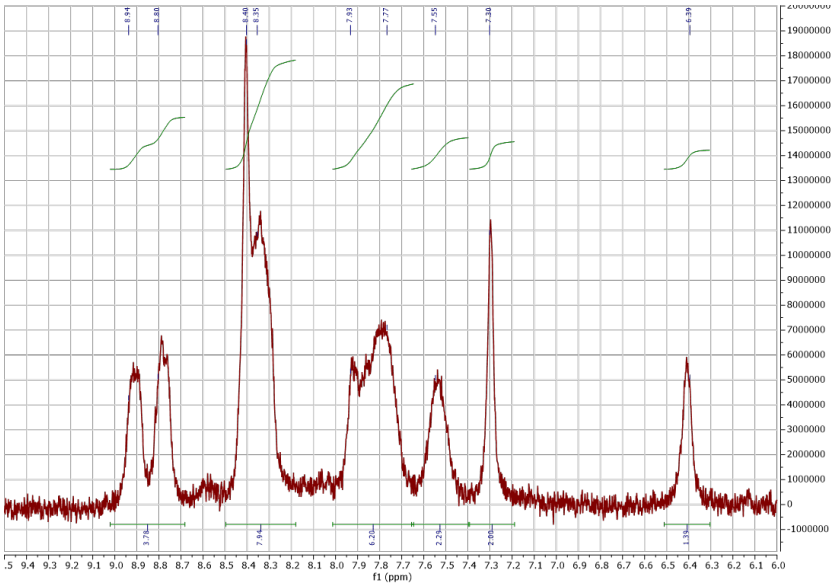
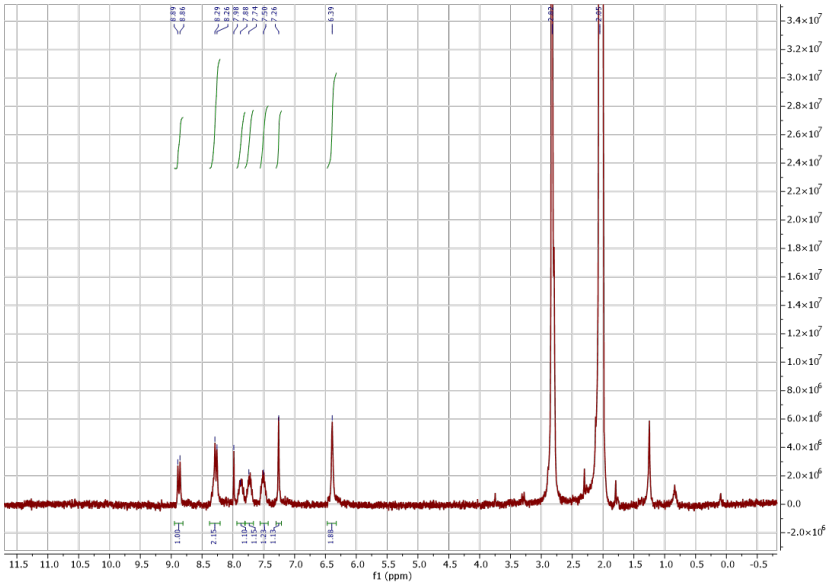


Figure S4: ^{1}H NMR spectrum of [Ru(phen)(phen-NH_2)$_2$](PF6)$_2$ in CD_3CO.



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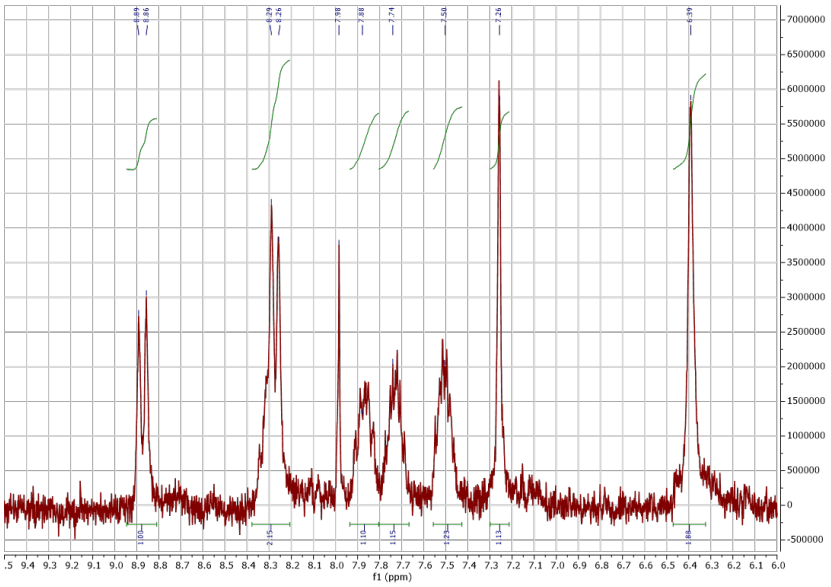
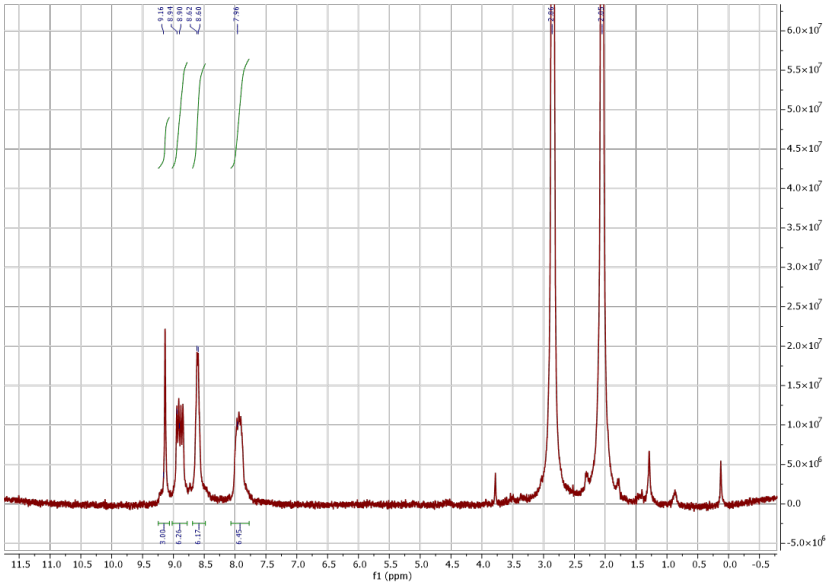


Figure S5: ^{1}H NMR spectrum of [Ru(phen-NH_2)$_3$](PF6)$_2$ in CD_3CO.



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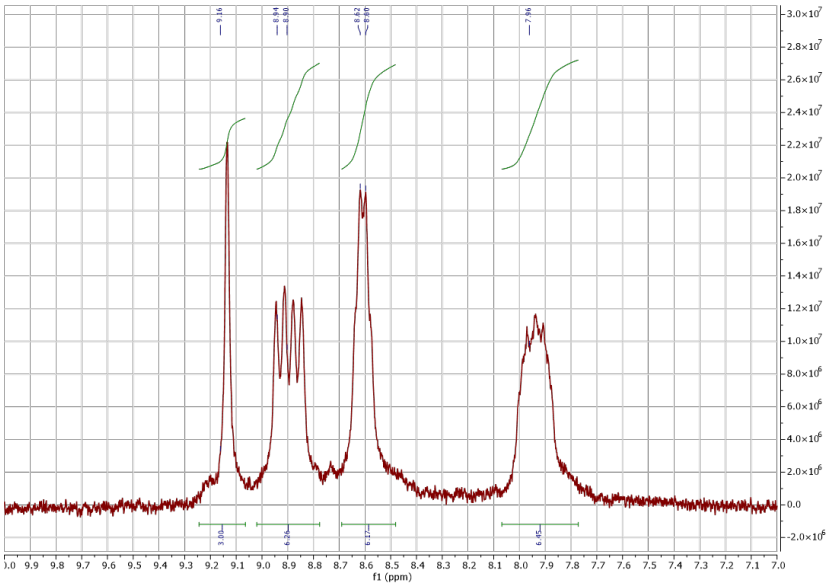


Figure S6: ^{1}H NMR spectrum of [Ru(phen-CN)$_3$](PF6)$_2$ in CD_3CO.

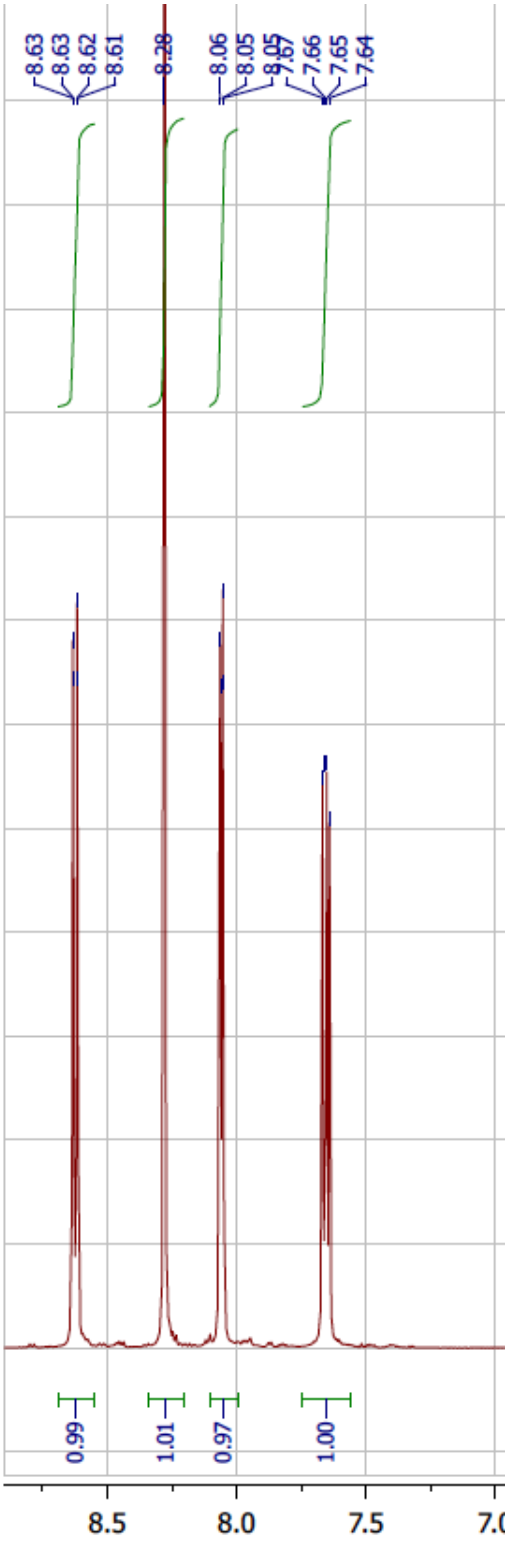


Figure S7: ^{1}H NMR spectrum of $[Ru(phen)_3](PF6)_2$ in CD_3CO.

S2 Electrochemical measurements

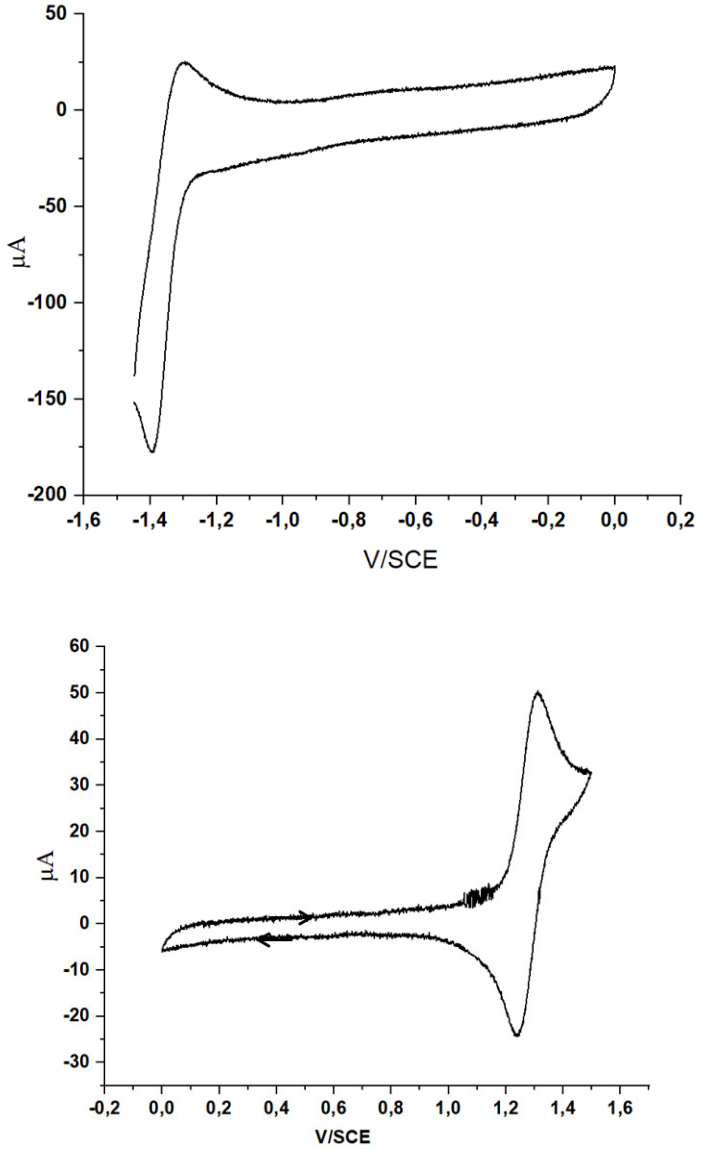


Figure S8: Cyclic voltammetry of complex $[Ru(phen)_3]^{2+}$.

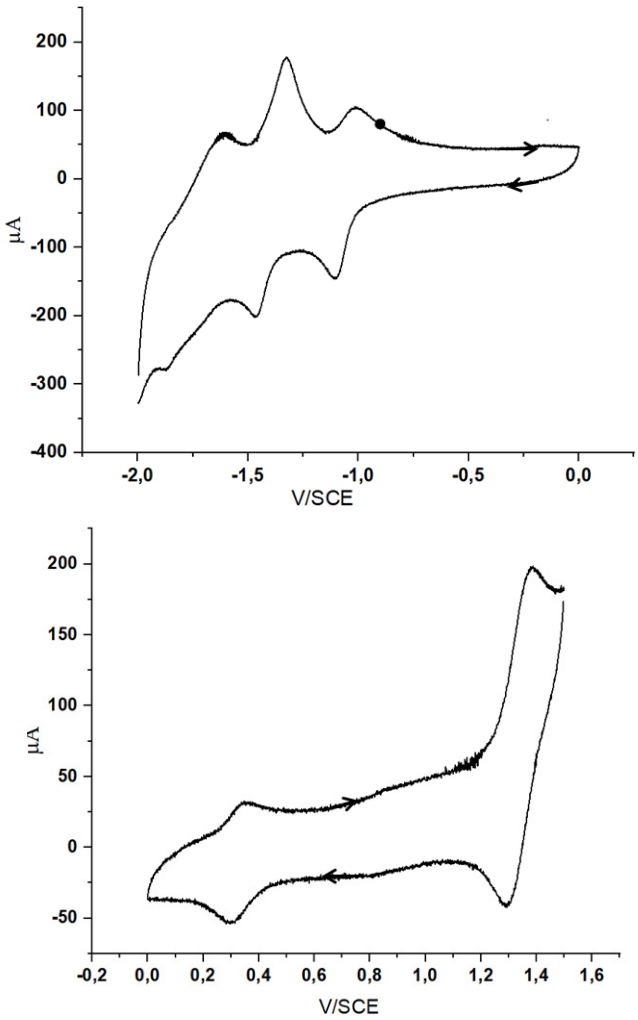


Figure S9: Cyclic voltammetry of complex $[Ru(phen)_2(phen\text{-}CN)]^{2+}$.

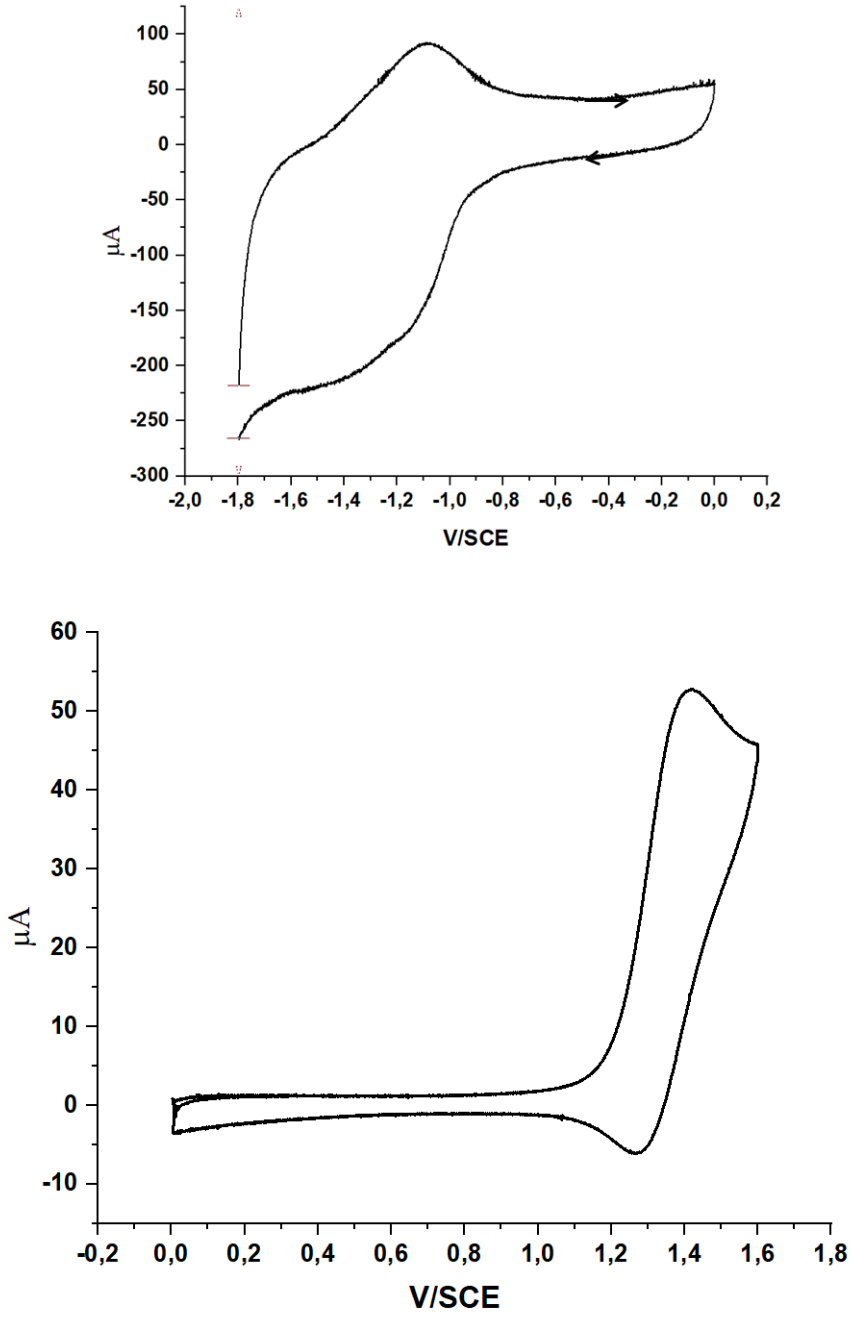


Figure S10: Cyclic voltammetry of complex $[Ru(phen\text{-}CN)_3]^{2+}$.

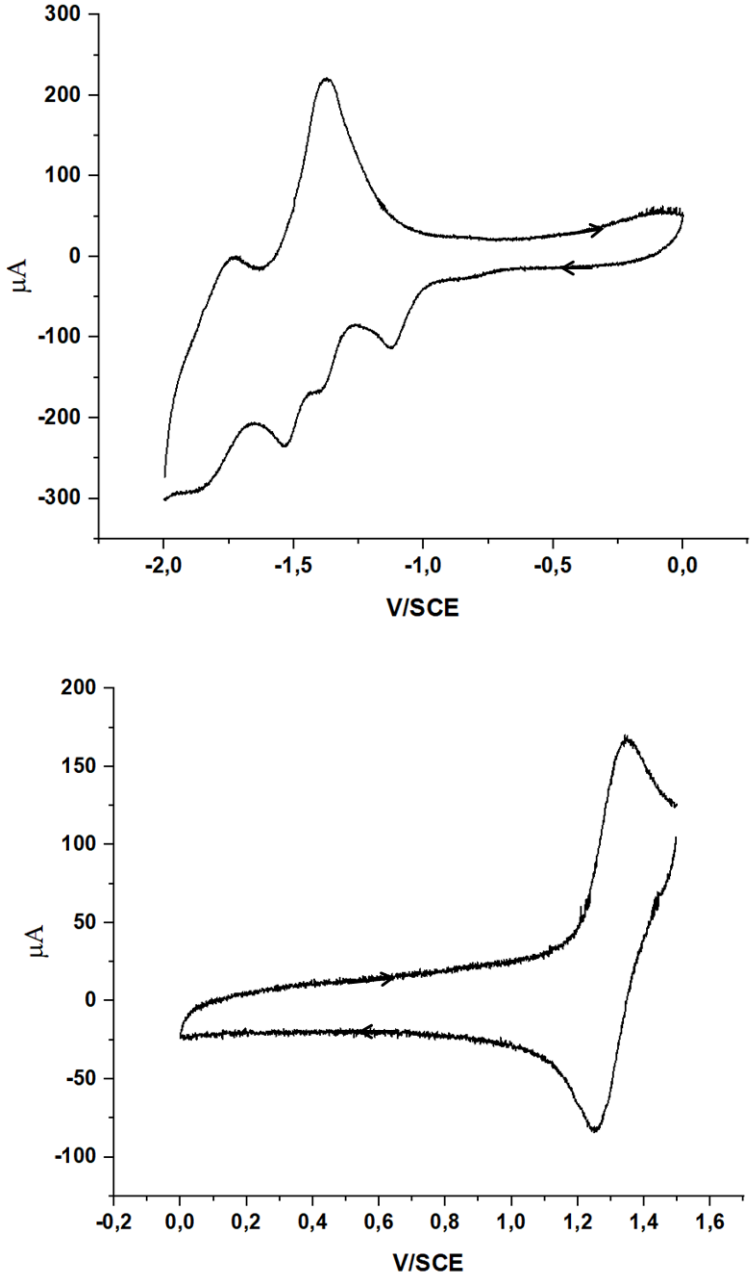


Figure S11: Cyclic voltammetry of complex $[Ru(phen)_2(phen\text{-}epoxy)]^{2+}$.

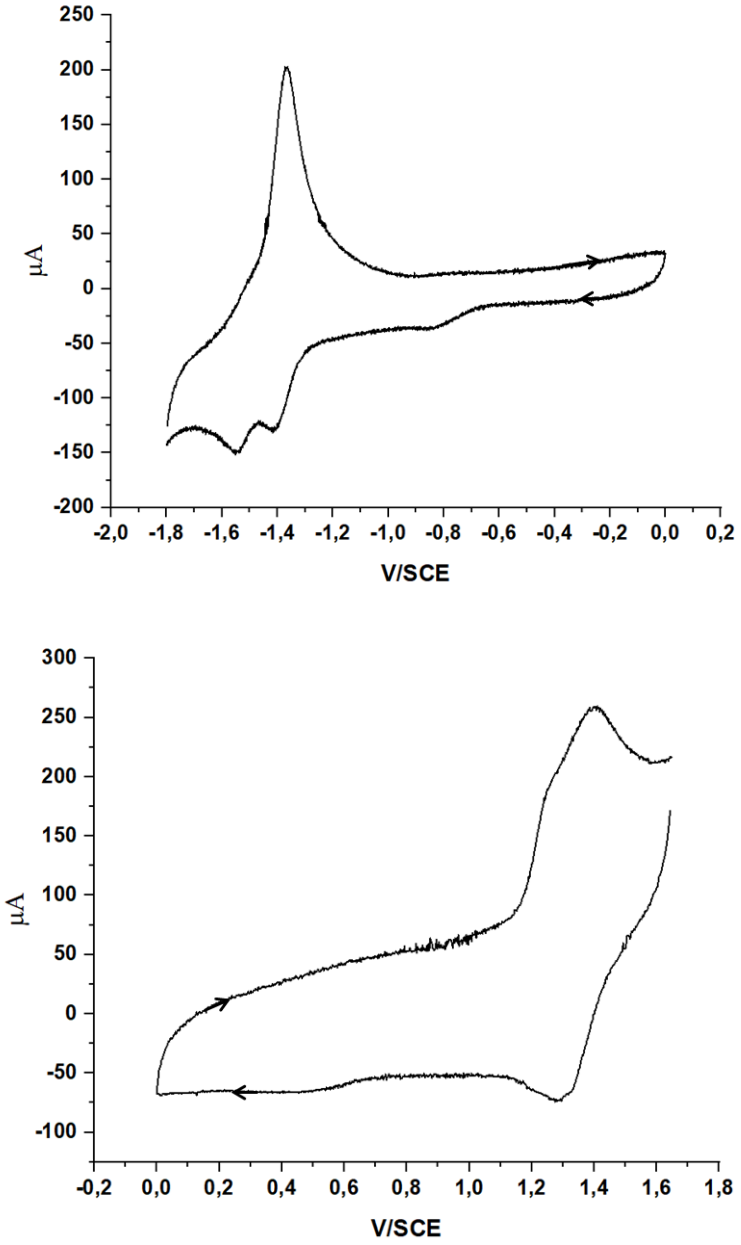


Figure S12: Cyclic voltammetry of complex $[Ru(phen)_2(phen\text{-}NH_2)]^{2+}$.

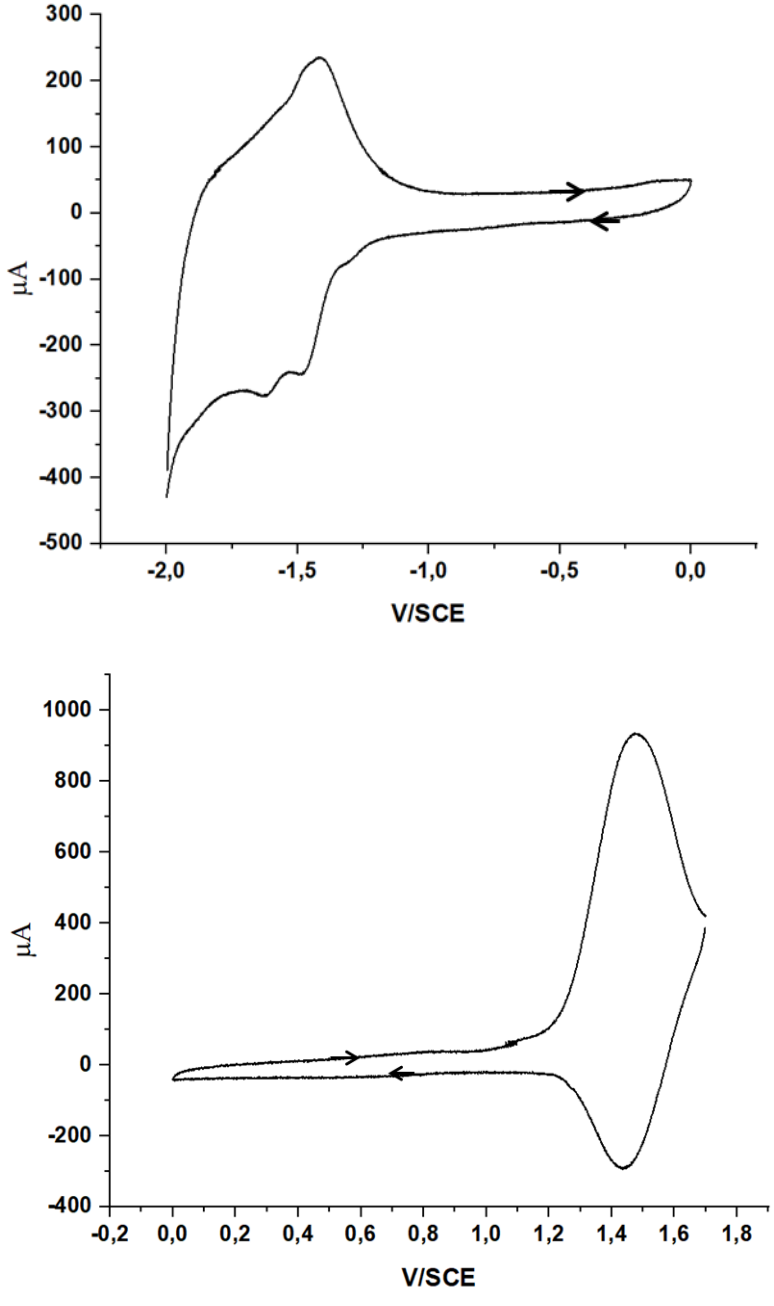


Figure S13: Cyclic voltammetry of complex $[Ru(phen\text{-}NH_2)_3]^{2+}$.

S3 Jablonski diagram

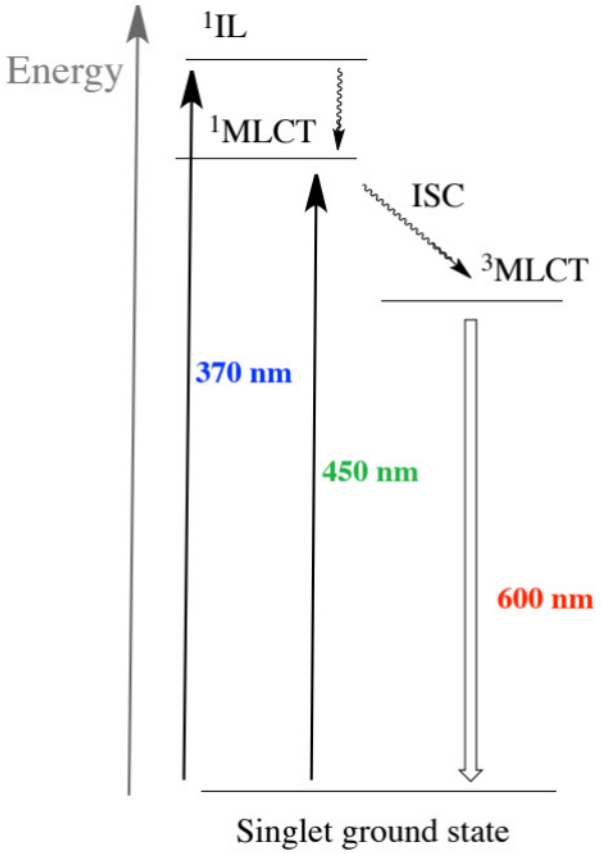


Figure S14: Simplified Jablonski diagram for Ru(II) complexes

S4 Influence of the phen → phen-X (C = CN, NH_2) substitution on the absorption spectrum of $[Ru(phen)_3]^{2+}$

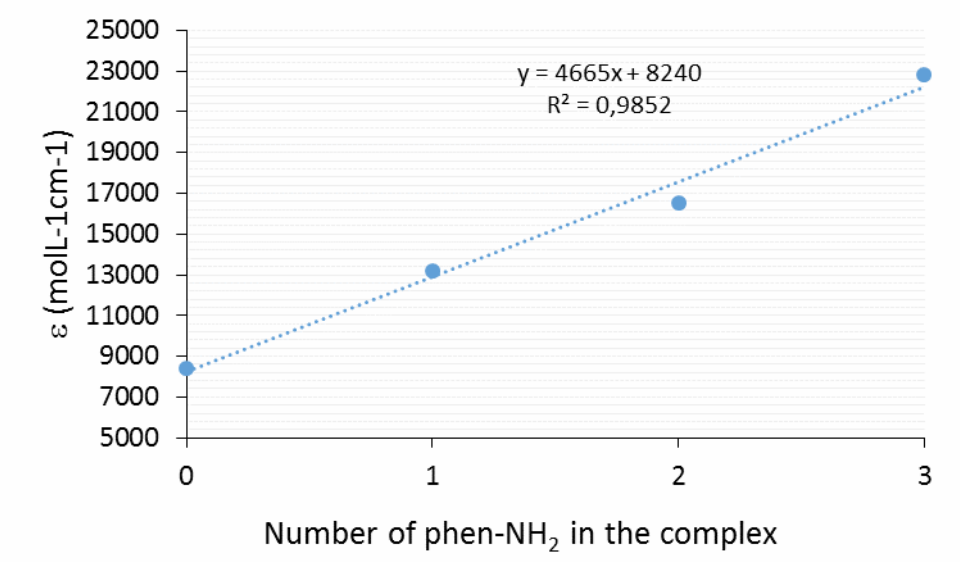


Figure S15: Evolution of the molar extinction coefficient of $[Ru(phen)_{3-n}(phen\text{-}NH_2)_n]^{2+}$ at 370 nm with the number n of phen-NH_2 ligand.

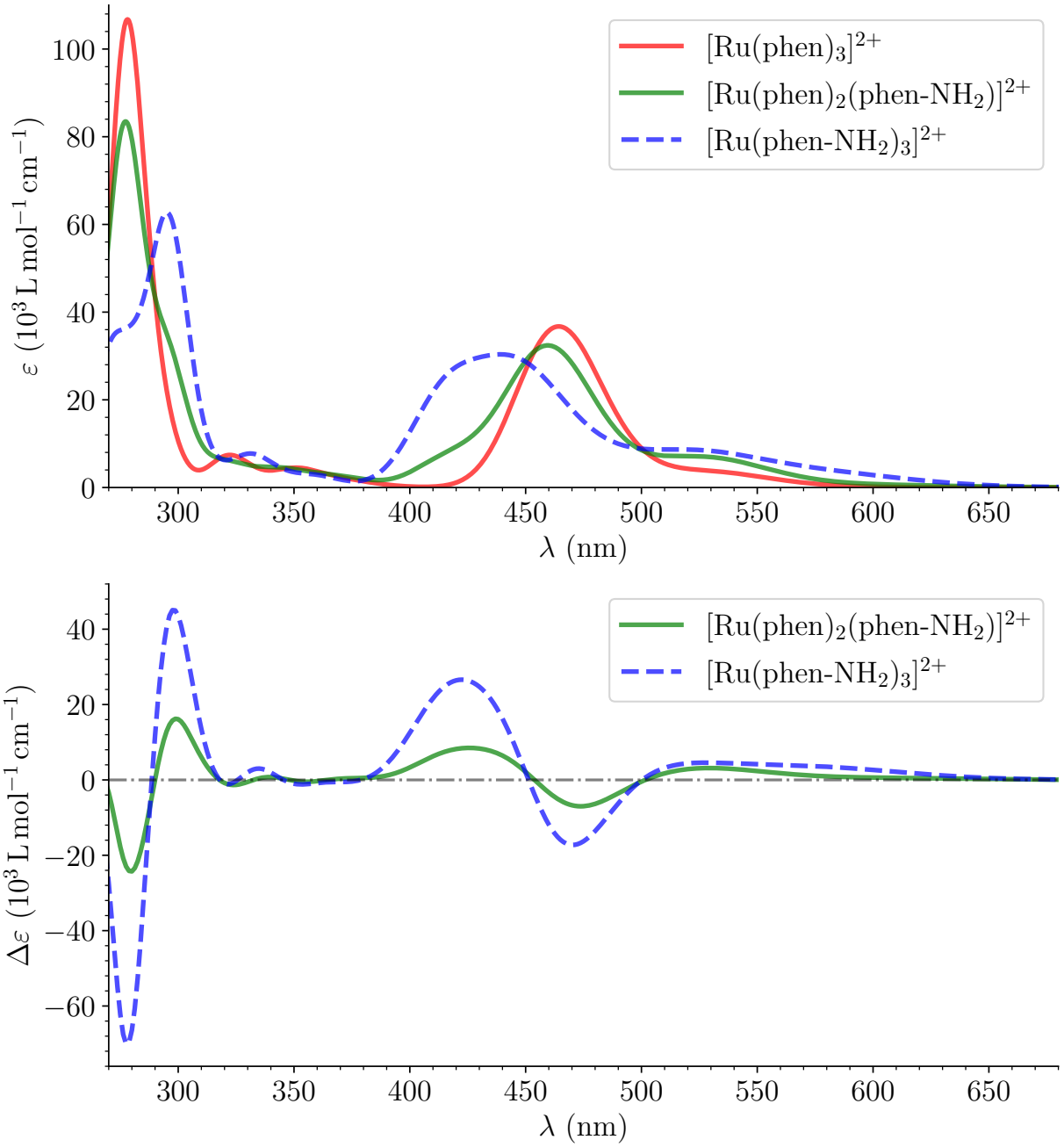


Figure S16: Calculated absorption spectra of $[Ru(phen)_3]^{2+}$, $[Ru(phen)_2(phen\text{-}NH_2)]^{2+}$ and $[Ru(phen\text{-}NH_2)_3]^{2+}$: (Top) comparison of the spectra, (Bottom) difference spectra with respect to the one of the reference complex $[Ru(phen)_3]^{2+}$.

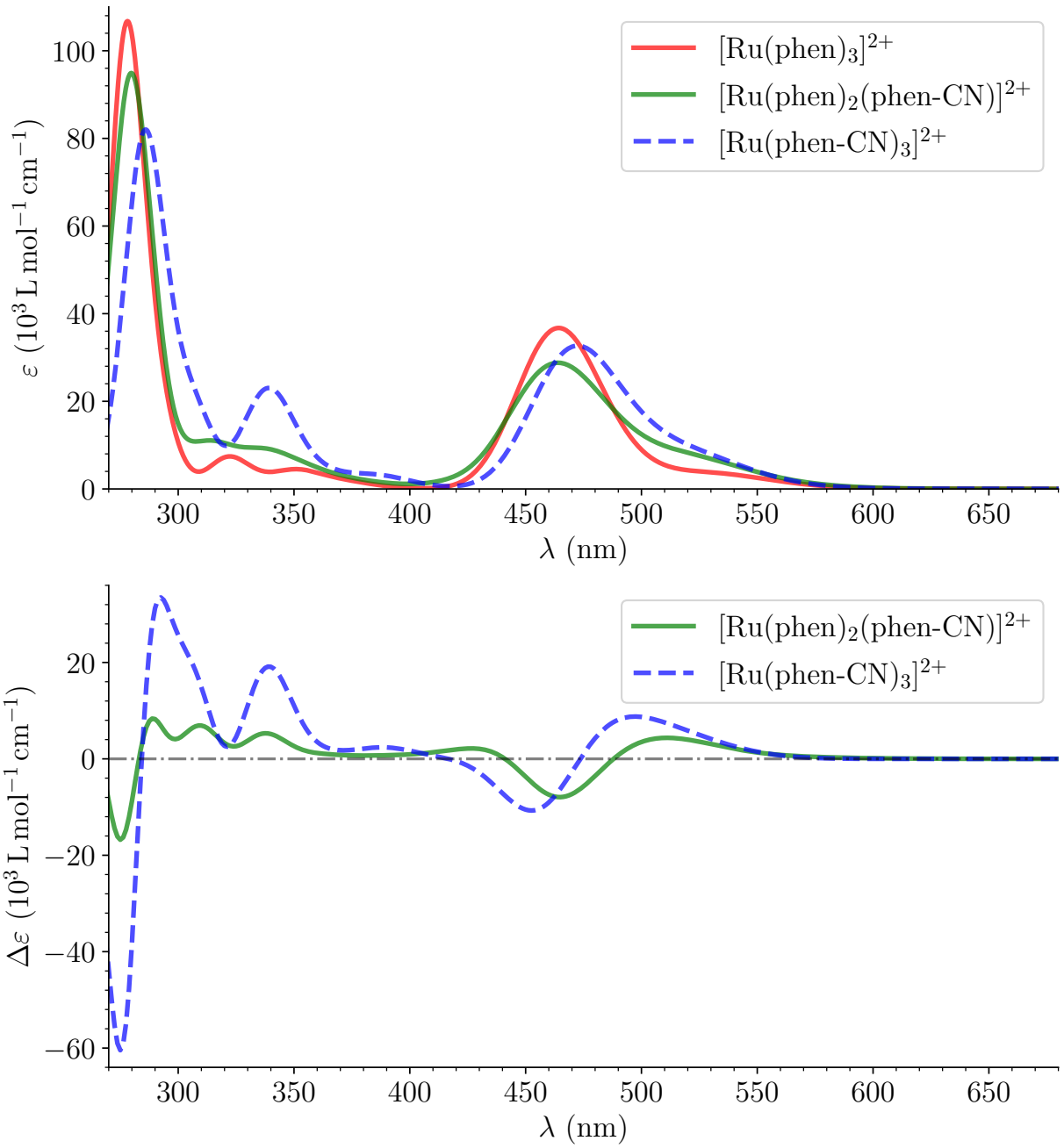


Figure S17: Calculated absorption spectra of $[Ru(phen)_3]^{2+}$, $[Ru(phen)_2(phen\text{-}CN)]^{2+}$ and $[Ru(phen\text{-}CN)_3]^{2+}$: (Top) comparison of the spectra, (Bottom) difference spectra with respect to the one of the reference complex $[Ru(phen)_3]^{2+}$.

S5 Influence of the solvent on the absorption and emission spectra of $[Ru(phen)_{3-x}(phen\text{-}NH_2)_x](PF_6)_2$ $(x = 1, 2, 3)$

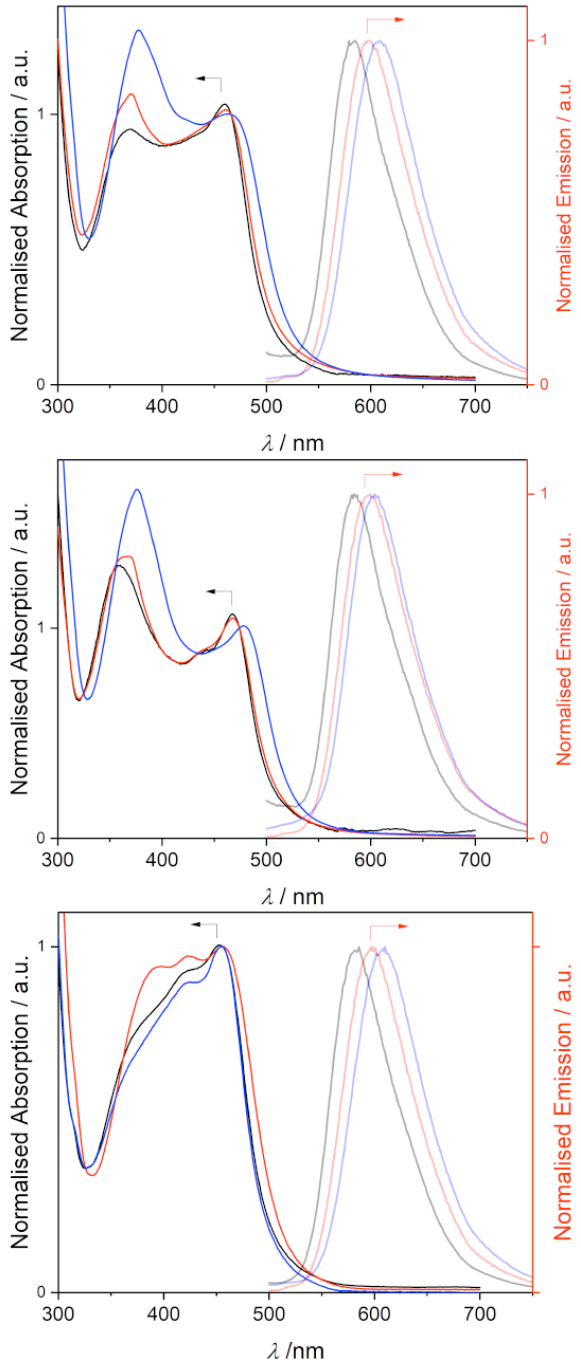


Figure S18: Absorption and emission spectra (λ_{exc} = 460 nm) in several solvents of $[Ru(phen)_2(phen\text{-}NH_2)](PF_6)_2$ (top), $[Ru(phen)(phen\text{-}NH_2)_2](PF_6)_2$ (middle) and $[Ru(phen\text{-}NH_2)_3](PF_6)_2$ (bottom). Spectra recorded in CH_2Cl_2 (black/grey), CH_3CN (red/light red) and in DMSO (blue/light blue).

S6 Time-Correlated Single Photon Counting (TCSPC) data

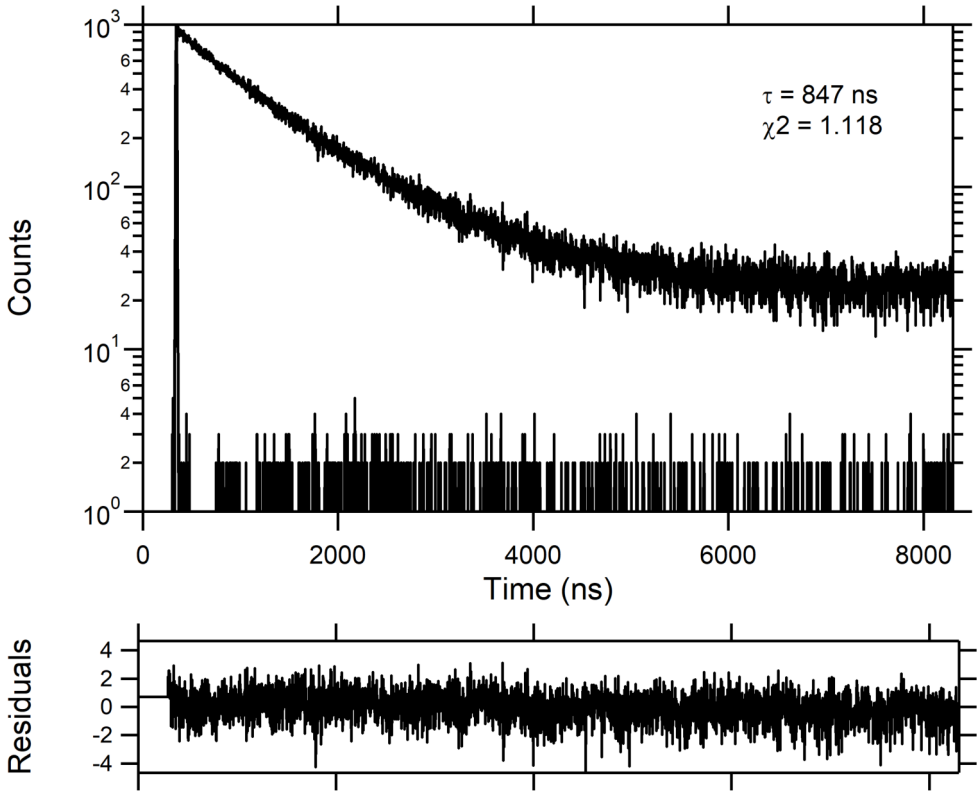


Figure S19: TCSPC data for $[Ru(phen)_2(phen\text{-}NH_2)](PF6)_2$ in deaerated CH_3CN.

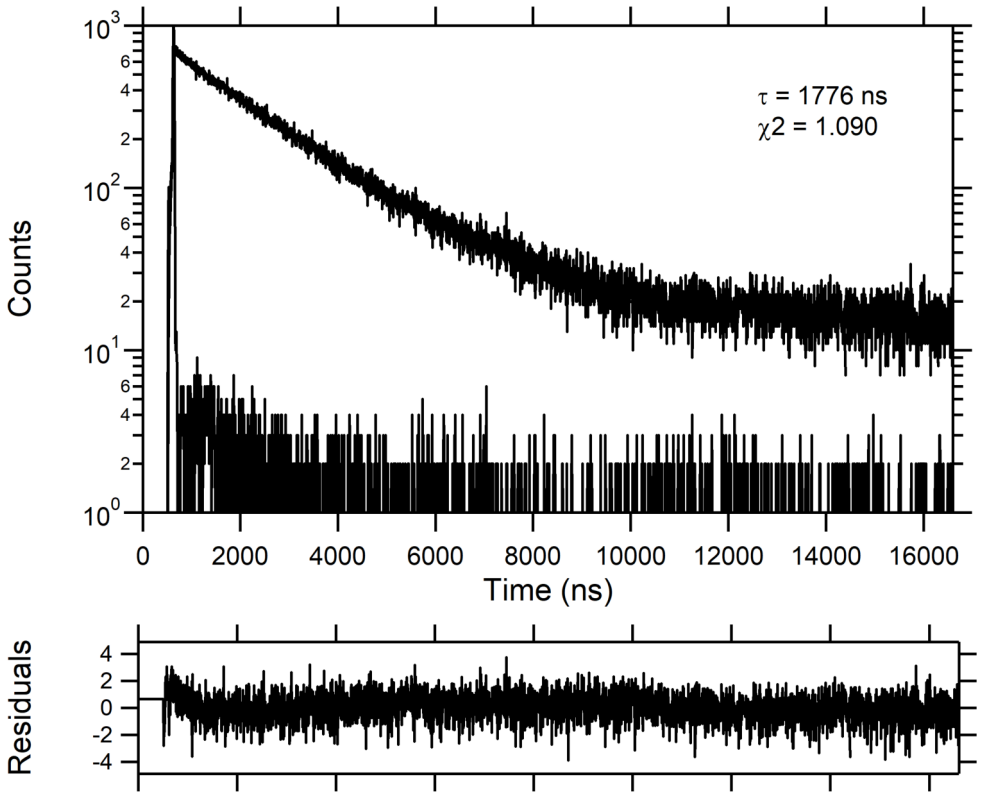


Figure S20: TCSPC data for [Ru(phen)$_2$(phen-CN)](PF6)$_2$ in deaerated CH_3CN.

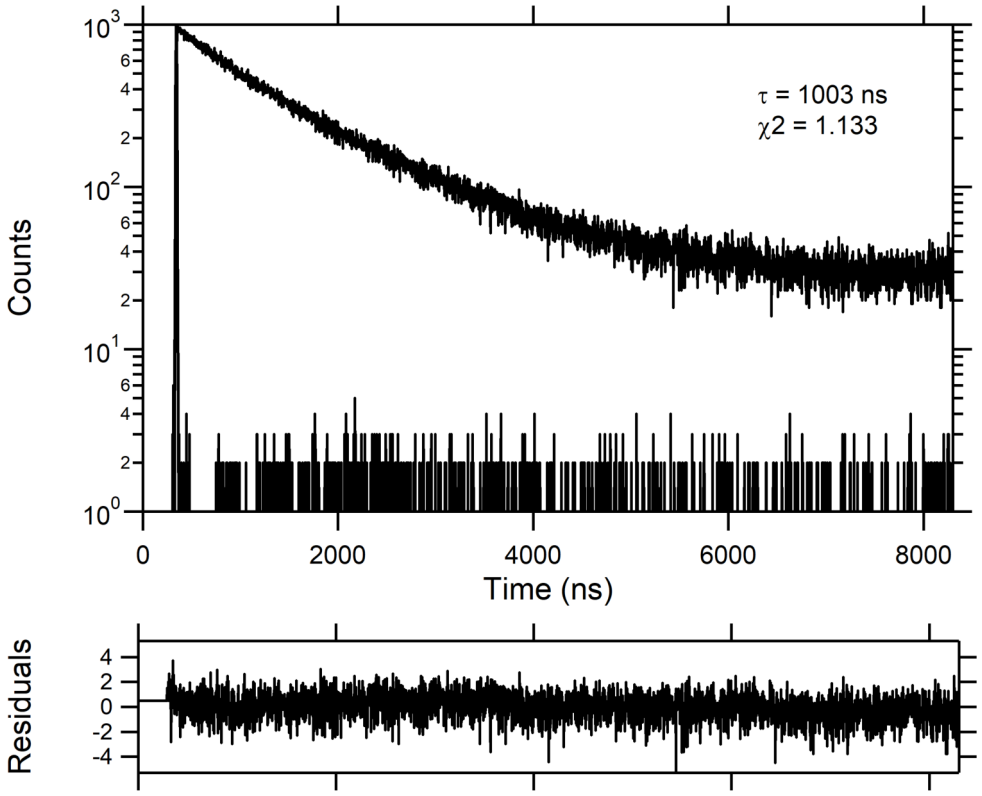


Figure S21: TCSPC data for [Ru(phen)(phen-NH_2)$_2$](PF6)$_2$ in deaerated CH_3CN.

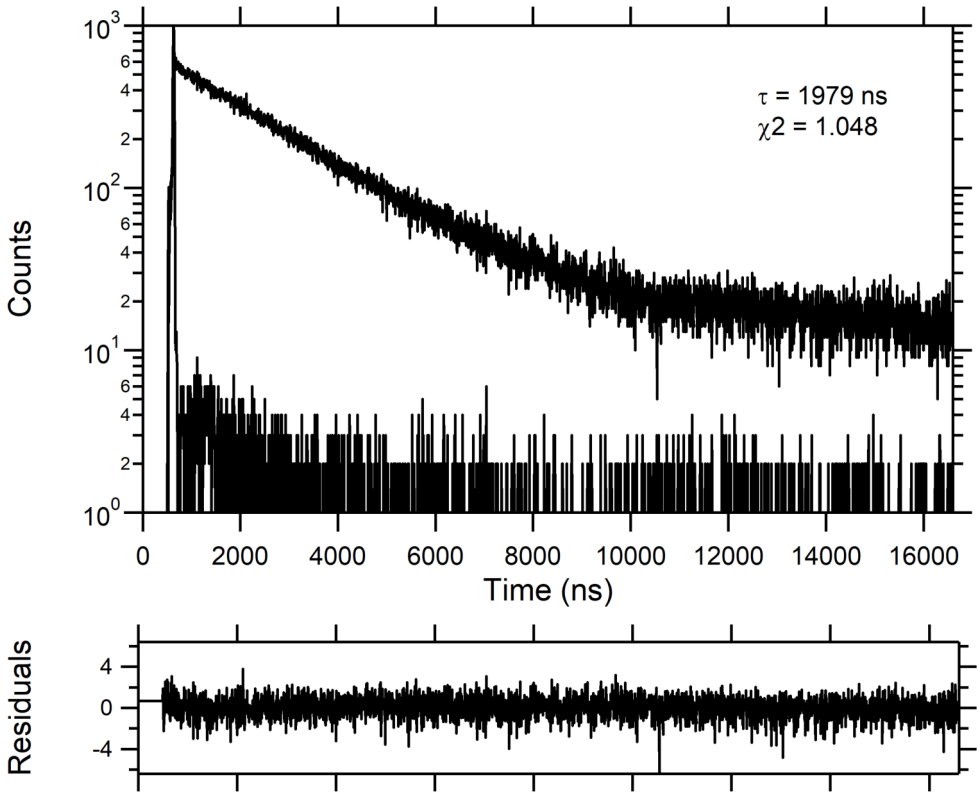


Figure S22: TCSPC data for $[Ru(phen\text{-}NH_2)_3](PF6)_2$ in deaerated CH_3CN.

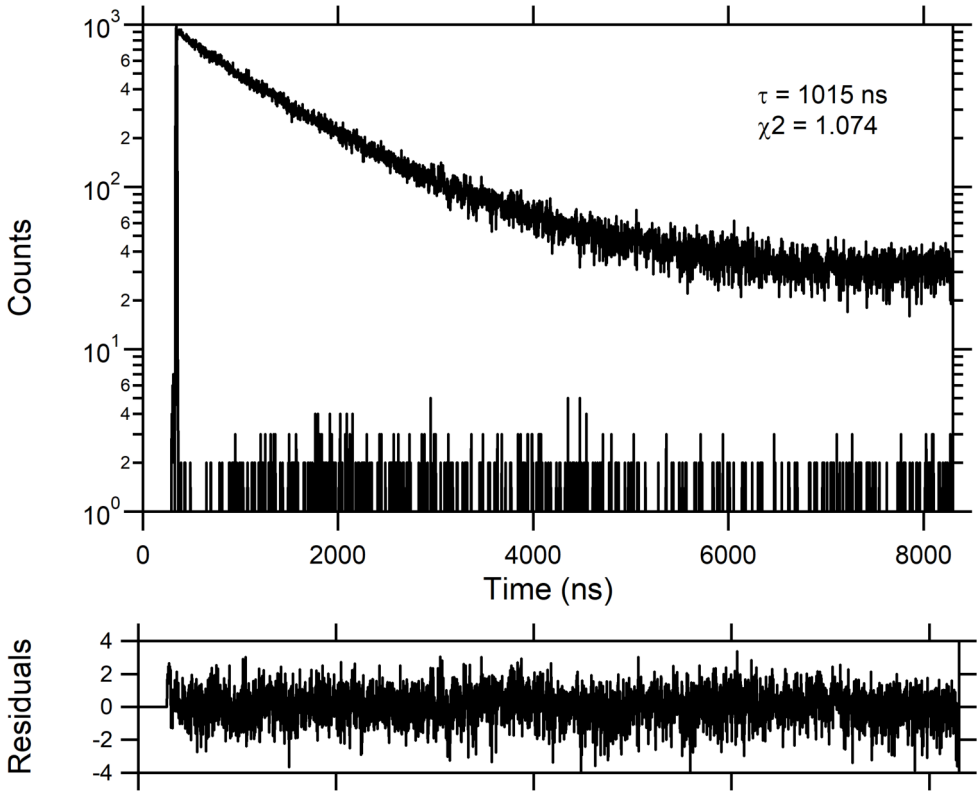
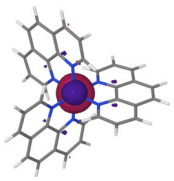
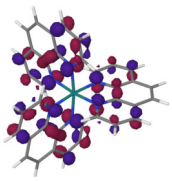


Figure S23: TCSPC data for$[Ru(phen\text{-}CN)_3](PF6)_2$ in deaerated CH_3CN.

S7 Computational results: $[Ru(phen)_3]^{2+}$

S7.1 HOMO-LUMO gap

HOMO	LUMO
	
$\varepsilon_{\mathrm{HOMO}} = -14.597$ eV	$\varepsilon_{\mathrm{LUMO}} = -12.467$ eV
$\Delta\varepsilon = 2.130$ eV	

S7.2 Calculated absorption spectrum

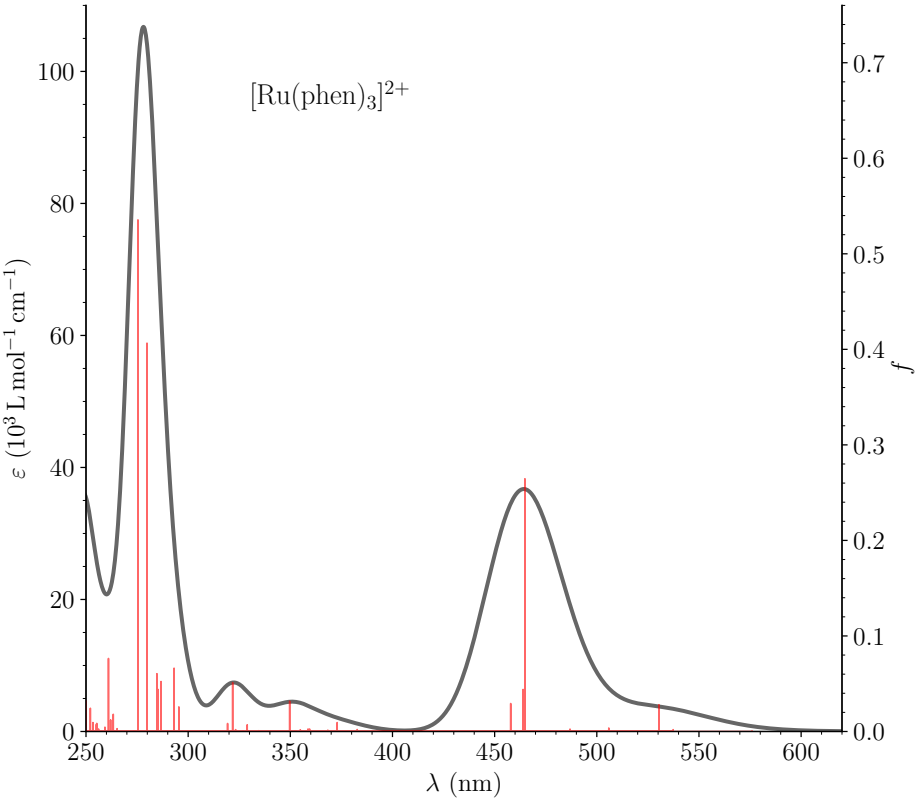
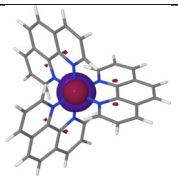
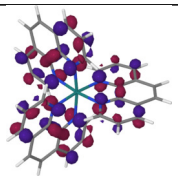
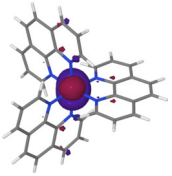
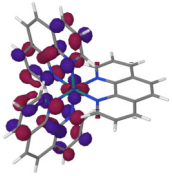
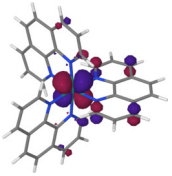
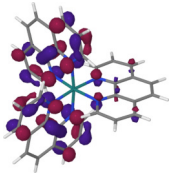
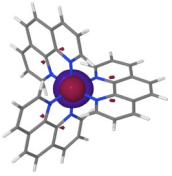
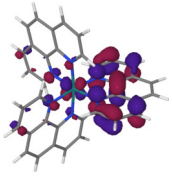
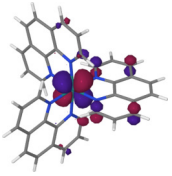
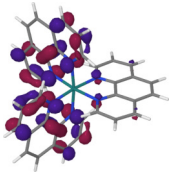
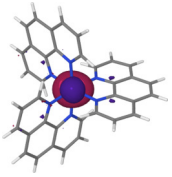
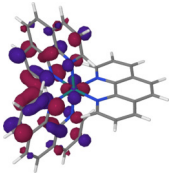
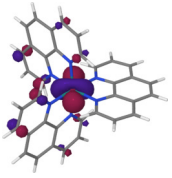
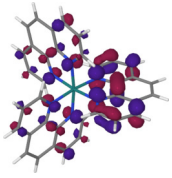
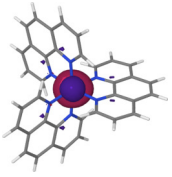
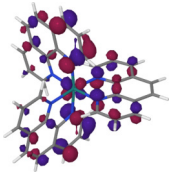
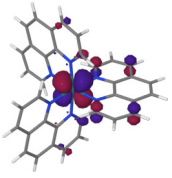
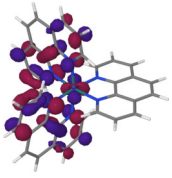


Figure S24: Absorption spectrum of $[Ru(phen)_3]^{2+}$ (C_2 symmetry) obtained by convoluting the calculated oscillators strengths f with Gaussian having a full-with-at-half-maximum of 2000 cm^{-1} (SAOP/TZ2P results).

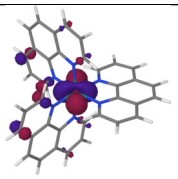
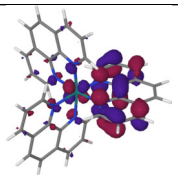
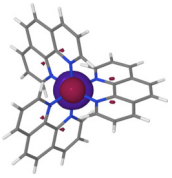
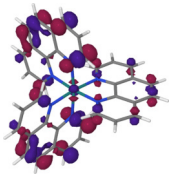
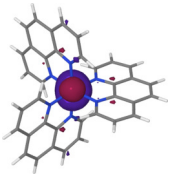
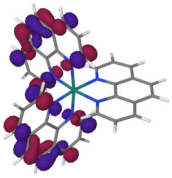
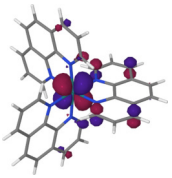
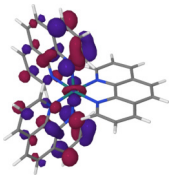
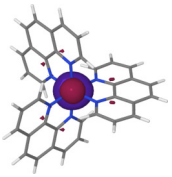
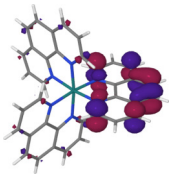
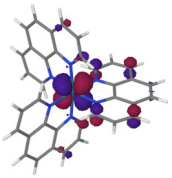
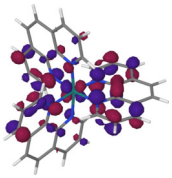
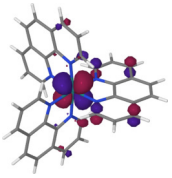
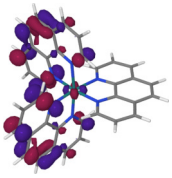
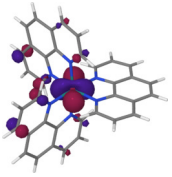
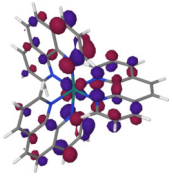
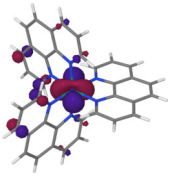
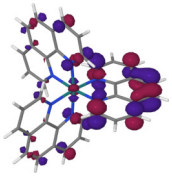
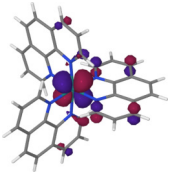
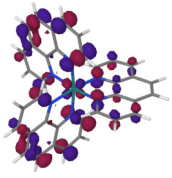
S7.3 Analysis of the electronic absorption spectrum

Table S1: Features of the $S_0 \rightarrow S_n$ electronic transition in $[Ru(phen)_3]^{2+}$ (C_2 symmetry): transition wavelength λ, oscillator strength f, description in terms of natural transition orbitals (NTO) with the weights ω of the NTO $\rightarrow$ NTO transitions (SAOP/TZ2P results)

Nr	Symm.	λ (nm)	f	NTO			
				(%)	occ.	$\rightarrow$	virt.
1	1^1B	575	0.001	99			
2	1^1A	538	0.003	68			
				31			
3	2^1B	535	0.001	90			
4	2^1A	531	0.011	60			
				39			
5	3^1B	530	0.016	81			
				15			
6	4^1B	514	0.000	51			

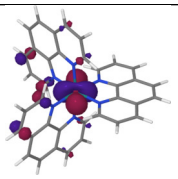
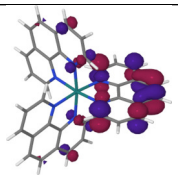
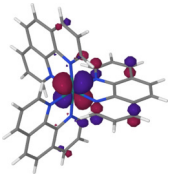
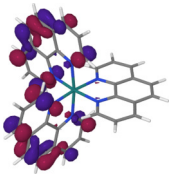
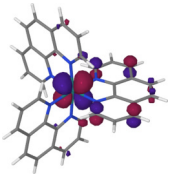
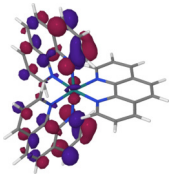
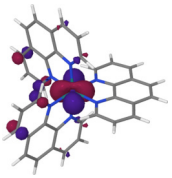
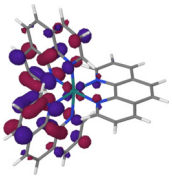
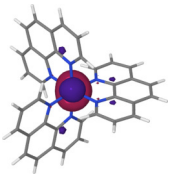
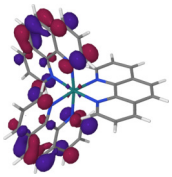
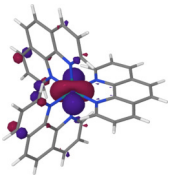
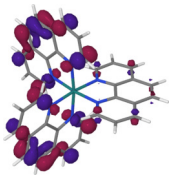
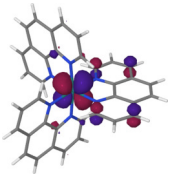
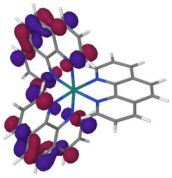
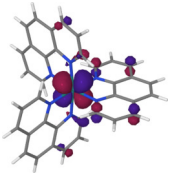
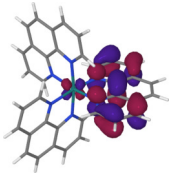
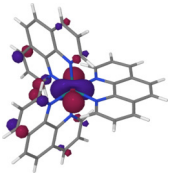
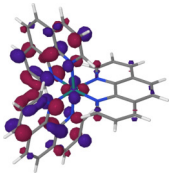
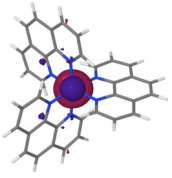
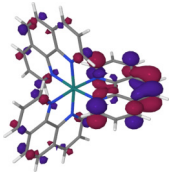
To be continued

Table S1 *continued*

Nr	Symm.	λ (nm)	f	NTO			
				(%)	occ.	→	virt.
				48			
7	3^1A	513	0.000	88			
8	5^1B	505	0.002	79			
				12			
9	4^1A	505	0.001	81			
				12			
10	6^1B	490	0.002	76			
				23			
11	5^1A	486	0.000	81			
				18			

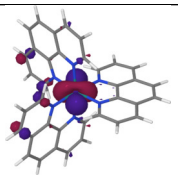
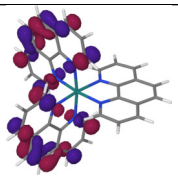
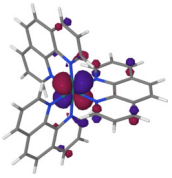
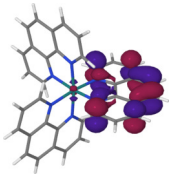
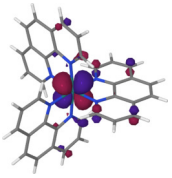
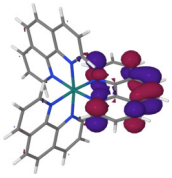
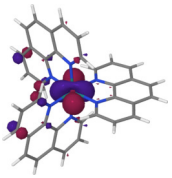
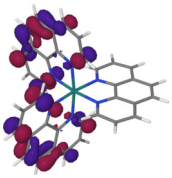
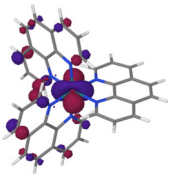
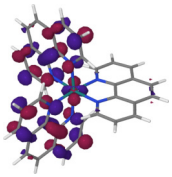
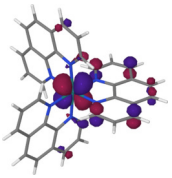
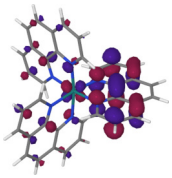
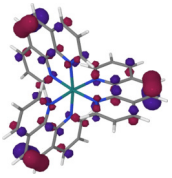
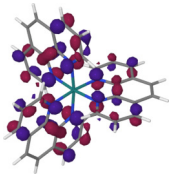
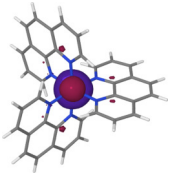
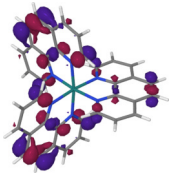
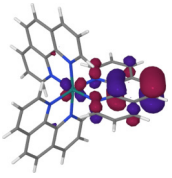
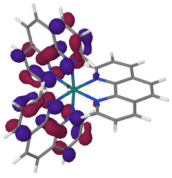
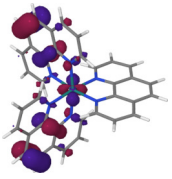
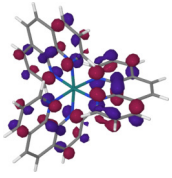
To be continued

Table S1 *continued*

Nr	Symm.	λ (nm)	f	NTO			
				(%)	occ.	→	virt.
12	6^1A	483	0.000	50			
				50			
13	7^1B	466	0.133	46			
				39			
				14			
14	7^1A	466	0.001	62			
				36			
15	8^1A	464	0.163	45			
				39			
				14			

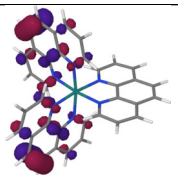
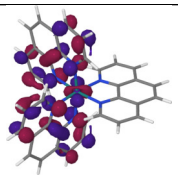
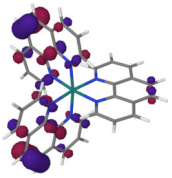
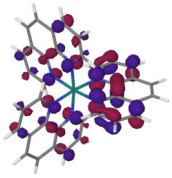
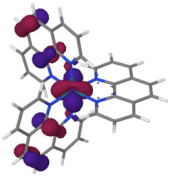
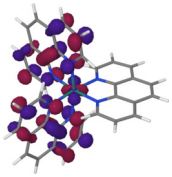
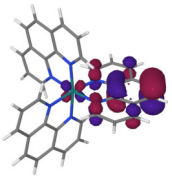
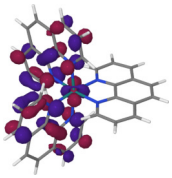
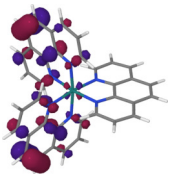
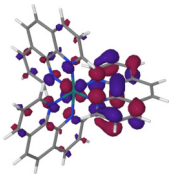
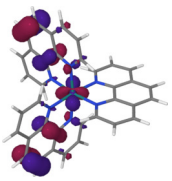
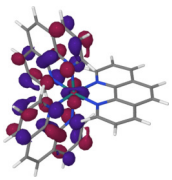
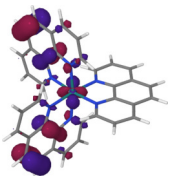
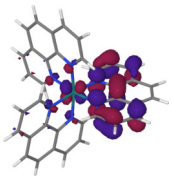
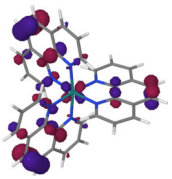
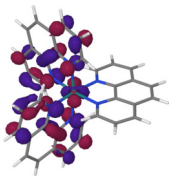
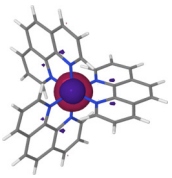
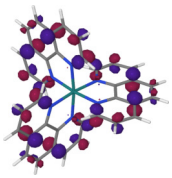
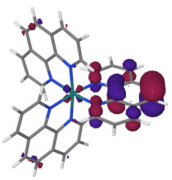
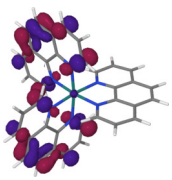
To be continued

Table S1 *continued*

Nr	Symm.	λ (nm)	f	NTO			
				(%)	occ.	→	virt.
16	8^1B	463	0.008	52			
				44			
17	9^1B	458	0.032	60			
				36			
18	9^1A	420	0.000	39			
				38			
				11			
				10			
19	10^1A	384	0.001	92			
20	10^1B	382	0.001	79			

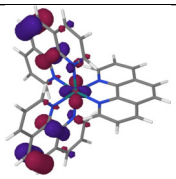
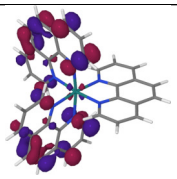
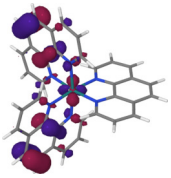
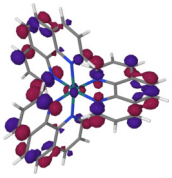
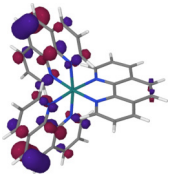
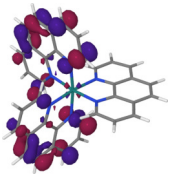
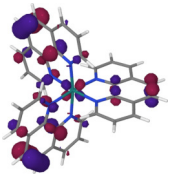
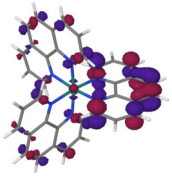
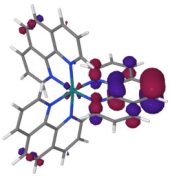
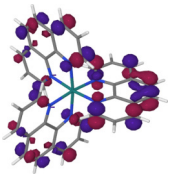
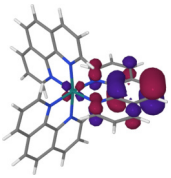
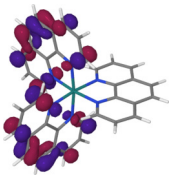
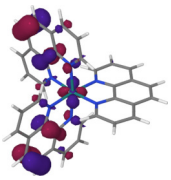
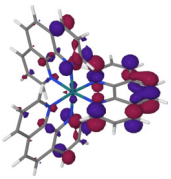
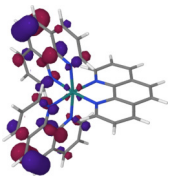
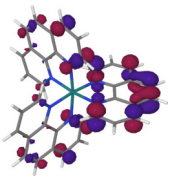
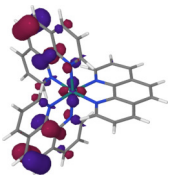
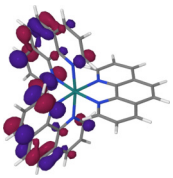
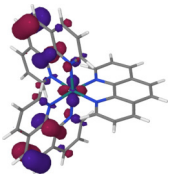
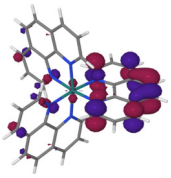
To be continued

Table S1 *continued*

Nr	Symm.	λ (nm)	f	NTO			
				(%)	occ.	→	virt.
				20			
21	11^1A	381	0.000	76			
				13			
22	11^1B	373	0.003	94			
23	12^1A	373	0.006	78			
				21			
24	12^1B	371	0.001	73			
				26			
25	13^1B	368	0.001	96			
26	14^1B	360	0.002	78			

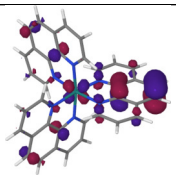
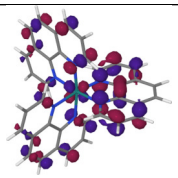
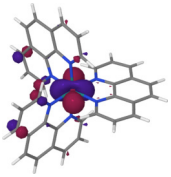
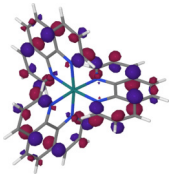
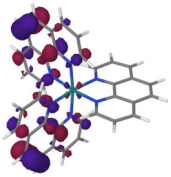
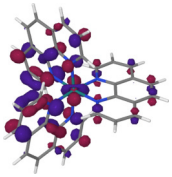
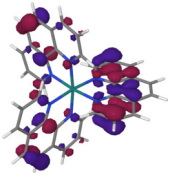
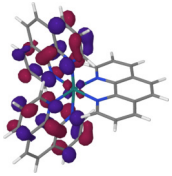
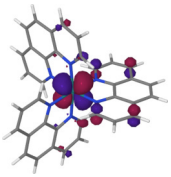
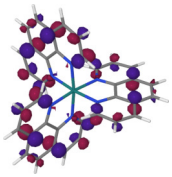
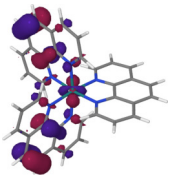
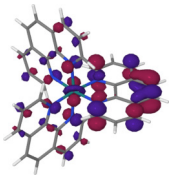
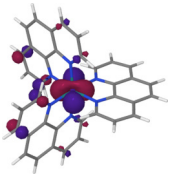
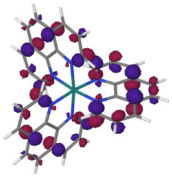
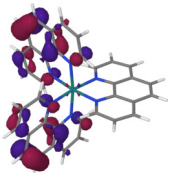
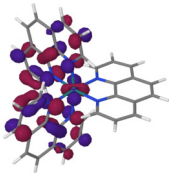
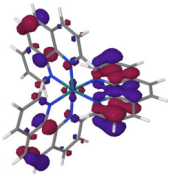
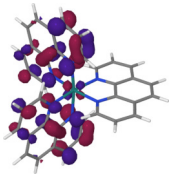
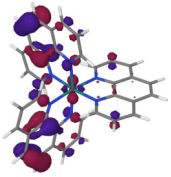
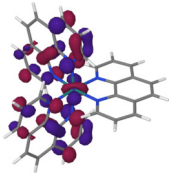
To be continued

Table S1 *continued*

Nr	Symm.	λ (nm)	f	NTO			
				(%)	occ.	→	virt.
				11			
27	13^1A	360	0.001	70			
				27			
28	15^1B	359	0.003	76			
				14			
29	14^1A	355	0.001	82			
				15			
30	16^1B	355	0.001	65			
				31			
31	15^1A	354	0.000	56			

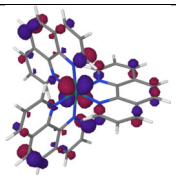
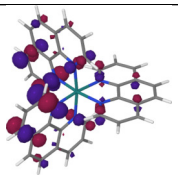
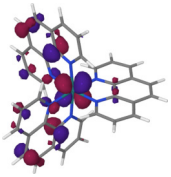
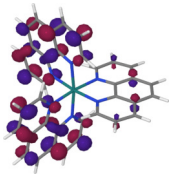
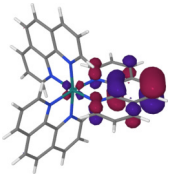
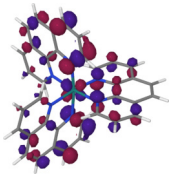
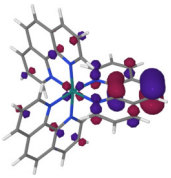
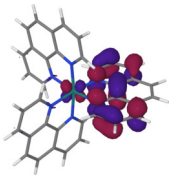
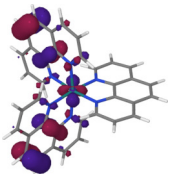
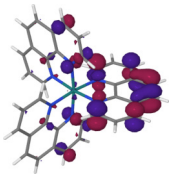
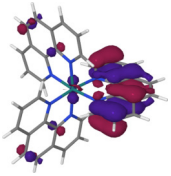
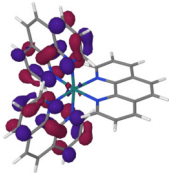
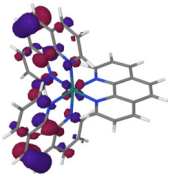
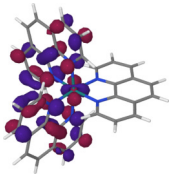
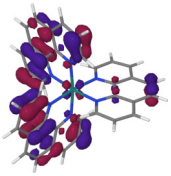
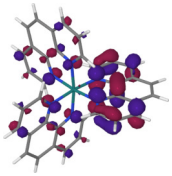
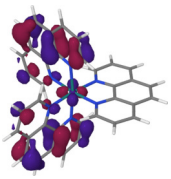
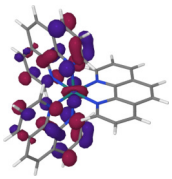
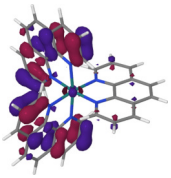
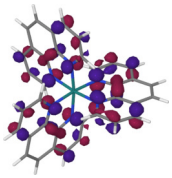
To be continued

Table S1 *continued*

Nr	Symm.	λ (nm)	f	NTO			
				(%)	occ.	→	virt.
				37			
32	17^1B	353	0.000	42			
				27			
				22			
33	16^1A	352	0.000	71			
				12			
34	18^1B	350	0.015	55			
				19			
				19			
35	17^1A	349	0.012	33			

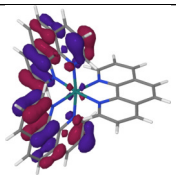
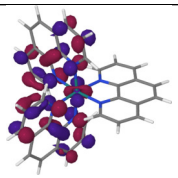
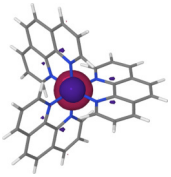
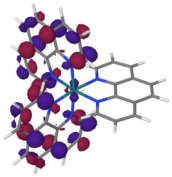
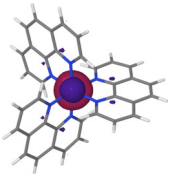
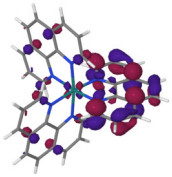
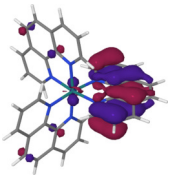
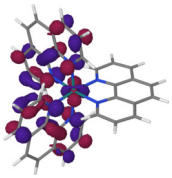
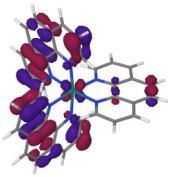
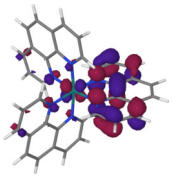
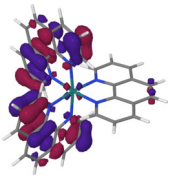
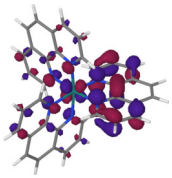
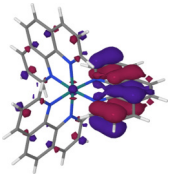
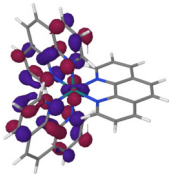
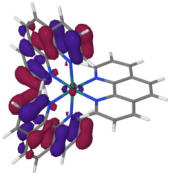
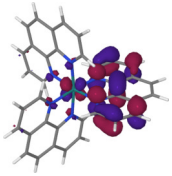
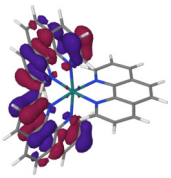
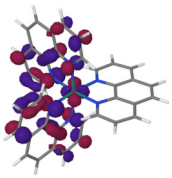
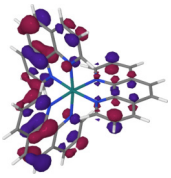
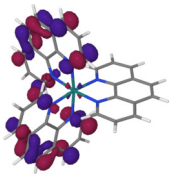
To be continued

Table S1 *continued*

Nr	Symm.	λ (nm)	f	NTO			
				(%)	occ.	→	virt.
				23			
				20			
				11			
36	18^1A	349	0.003	53			
				28			
37	19^1B	344	0.000	82			
				12			
38	19^1A	343	0.000	71			
				18			
39	20^1B	341	0.000	71			

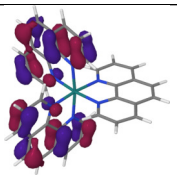
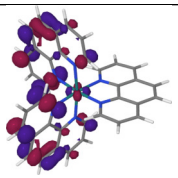
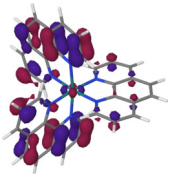
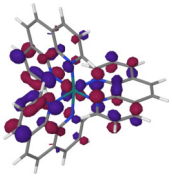
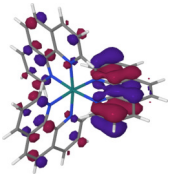
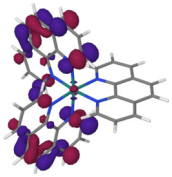
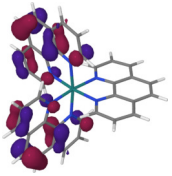
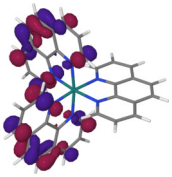
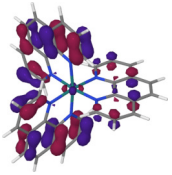
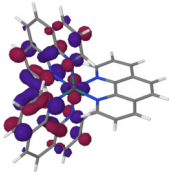
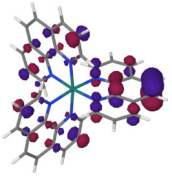
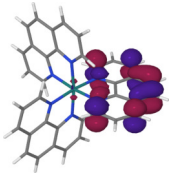
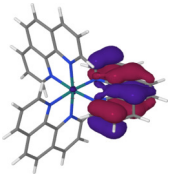
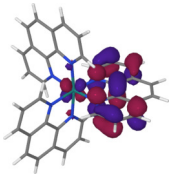
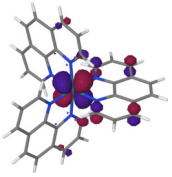
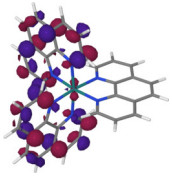
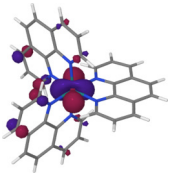
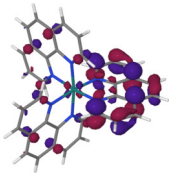
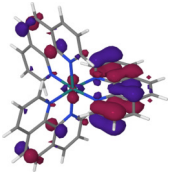
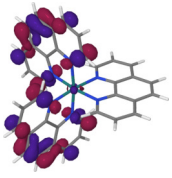
To be continued

Table S1 *continued*

Nr	Symm.	λ (nm)	f	NTO			
				(%)	occ.	→	virt.
				21			
40	20^1A	339	0.000	94			
41	21^1B	338	0.000	94			
42	21^1A	335	0.000	75			
				22			
43	22^1A	335	0.000	58			
				41			
44	22^1B	334	0.001	72			
				25			
45	23^1B	329	0.003	38			

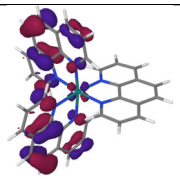
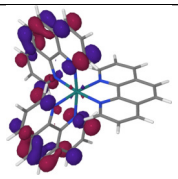
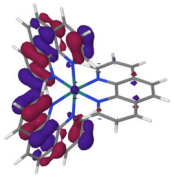
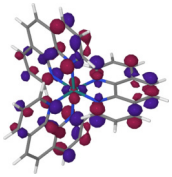
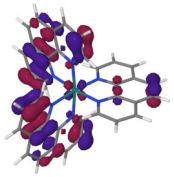
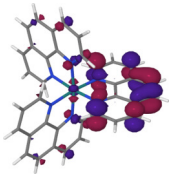
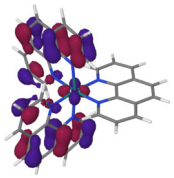
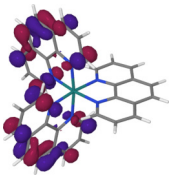
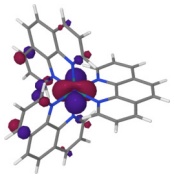
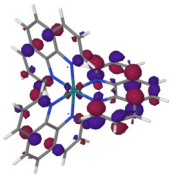
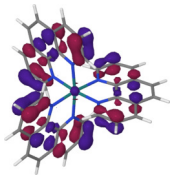
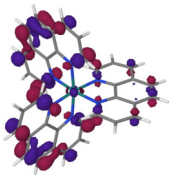
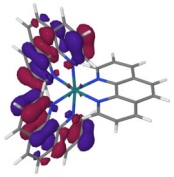
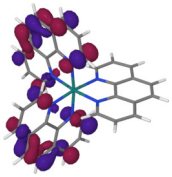
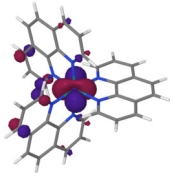
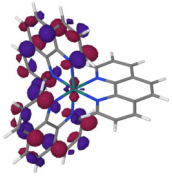
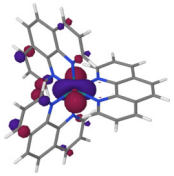
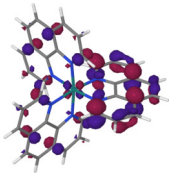
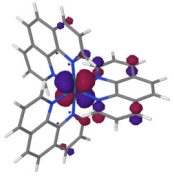
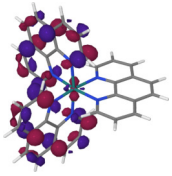
To be continued

Table S1 *continued*

Nr	Symm.	λ (nm)	f	NTO			
				(%)	occ.	→	virt.
				34			
				11			
46	23^1A	329	0.000	54			
				27			
				11			
47	24^1B	328	0.004	64			
				17			
48	25^1B	327	0.001	52			
				32			
49	24^1A	324	0.002	59			

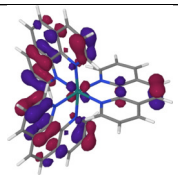
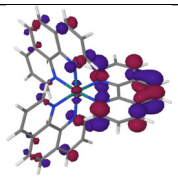
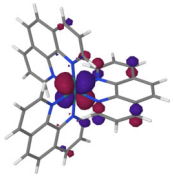
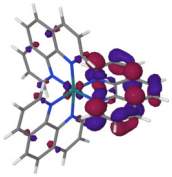
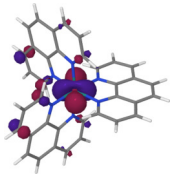
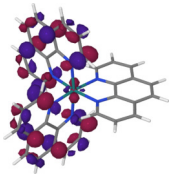
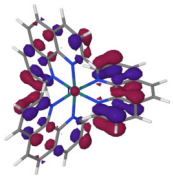
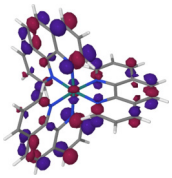
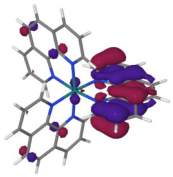
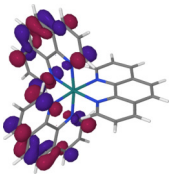
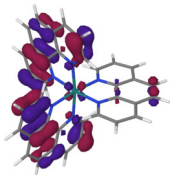
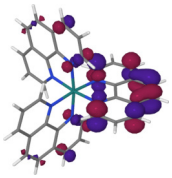
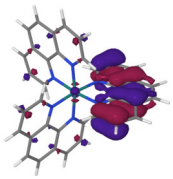
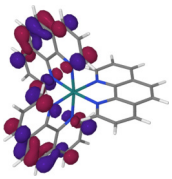
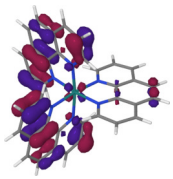
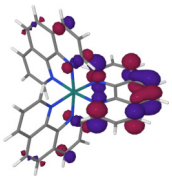
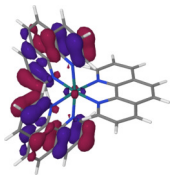
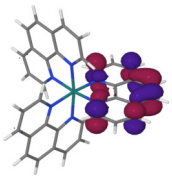
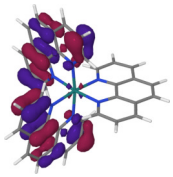
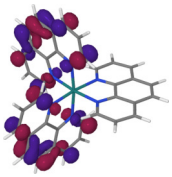
To be continued

Table S1 *continued*

Nr	Symm.	λ (nm)	f	NTO			
				(%)	occ.	→	virt.
				19			
				15			
50	26^1B	323	0.000	52			
				17			
				15			
51	25^1A	322	0.005	51			
				17			
				17			
52	27^1B	322	0.026	42			
				29			

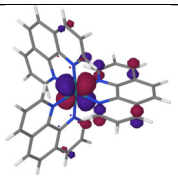
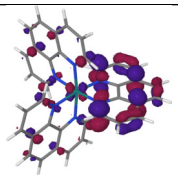
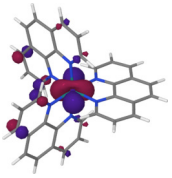
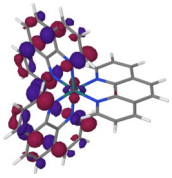
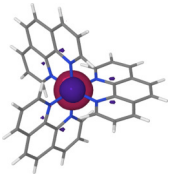
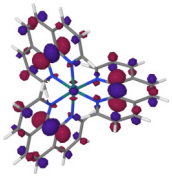
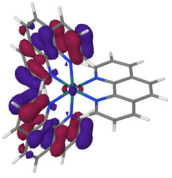
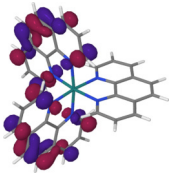
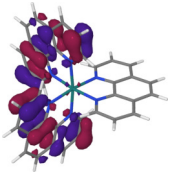
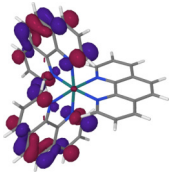
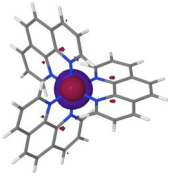
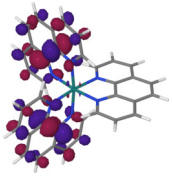
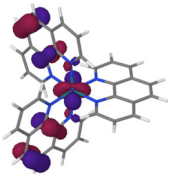
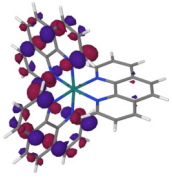
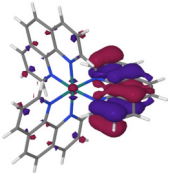
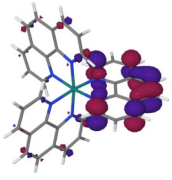
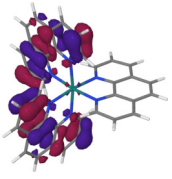
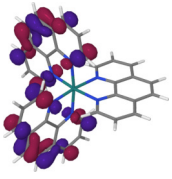
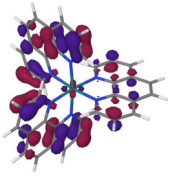
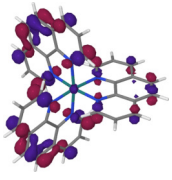
To be continued

Table S1 *continued*

Nr	Symm.	λ (nm)	f	NTO			
				(%)	occ.	→	virt.
				14			
53	26^1A	322	0.024	34			
				32			
				20			
54	28^1B	321	0.000	65			
				30			
55	29^1B	319	0.003	55			
				44			
56	27^1A	319	0.003	82			
				16			

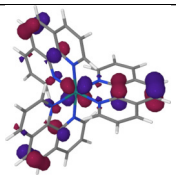
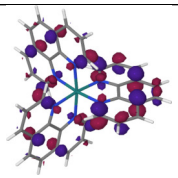
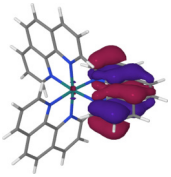
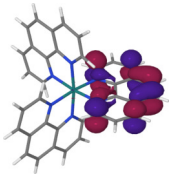
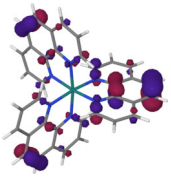
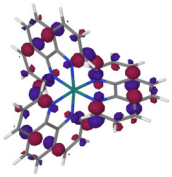
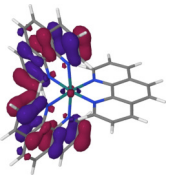
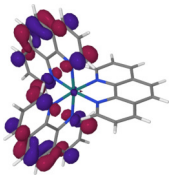
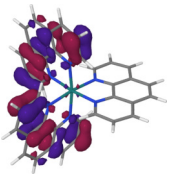
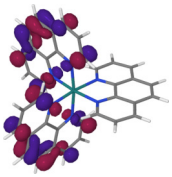
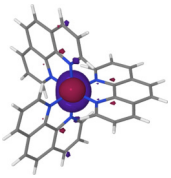
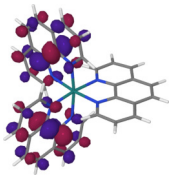
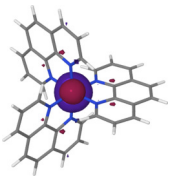
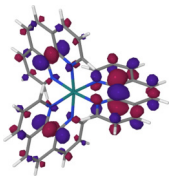
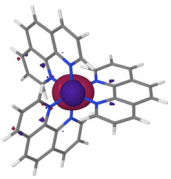
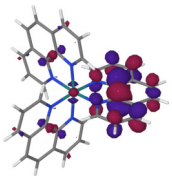
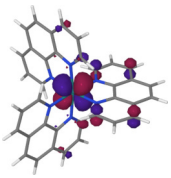
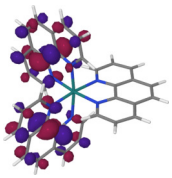
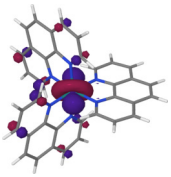
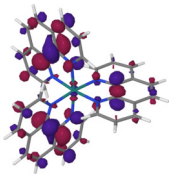
To be continued

Table S1 *continued*

Nr	Symm.	λ (nm)	f	NTO			
				(%)	occ.	→	virt.
57	28^1A	312	0.000	43			
				34			
				14			
58	30^1B	295	0.012	39			
				22			
				18			
				12			
59	29^1A	295	0.017	35			
				17			
				15			

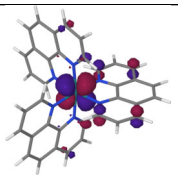
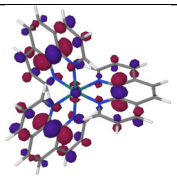
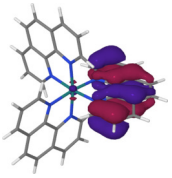
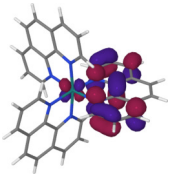
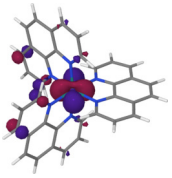
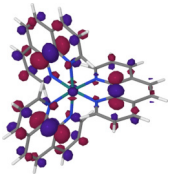
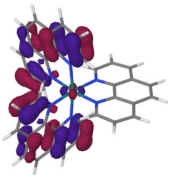
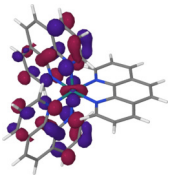
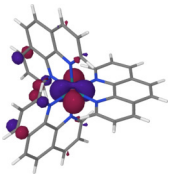
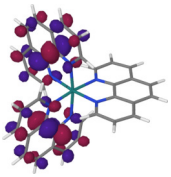
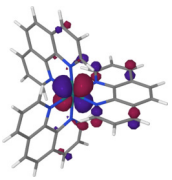
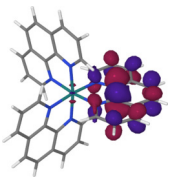
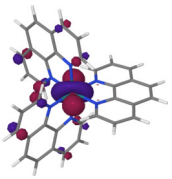
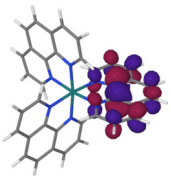
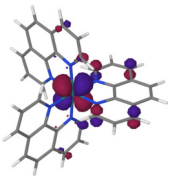
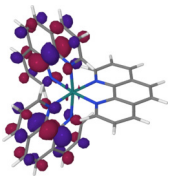
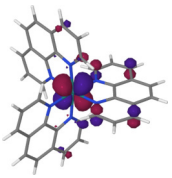
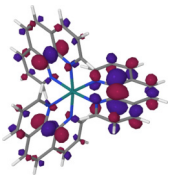
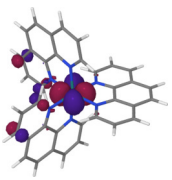
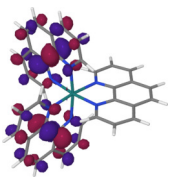
To be continued

Table S1 *continued*

Nr	Symm.	λ (nm)	f	NTO			
				(%)	occ.	→	virt.
				12			
60	30^1A	295	0.001	36			
				19			
				16			
				15			
61	31^1B	293	0.030	75			
62	31^1A	292	0.030	81			
63	32^1A	290	0.000	51			
				23			
				22			

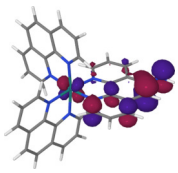
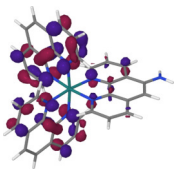
To be continued

Table S1 *continued*

Nr	Symm.	λ (nm)	f	NTO			
				(%)	occ.	→	virt.
64	32^1B	287	0.023	62			
				11			
65	33^1A	287	0.025	62			
				12			
66	33^1B	285	0.031	72			
				17			
67	34^1A	285	0.022	53			
				42			
68	34^1B	285	0.045	75			
				15			

S8 Computational results: $[Ru(phen)_2(phen\text{-}NH_2)]^{2+}$

S8.1 HOMO-LUMO gap

HOMO	LUMO
	
$\varepsilon_{HOMO} = -14.343$ eV	$\varepsilon_{LUMO} = -12.330$ eV
$\Delta\varepsilon = 2.013$ eV	

S8.2 Calculated absorption spectrum

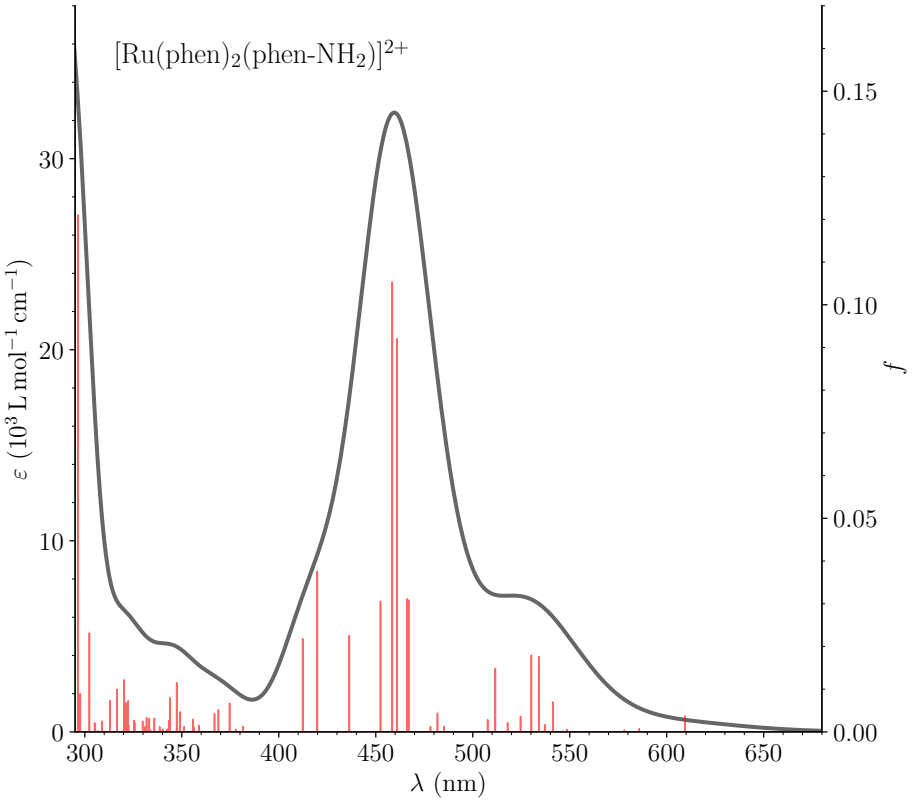
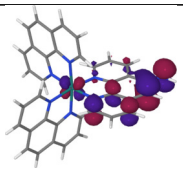
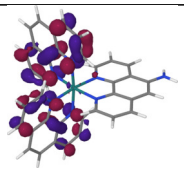
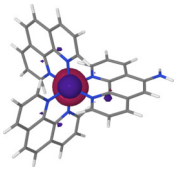
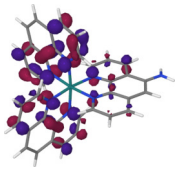
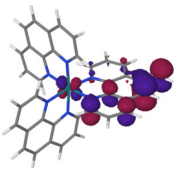
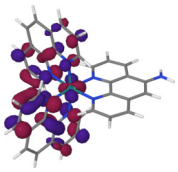
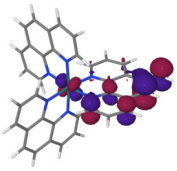
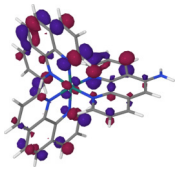
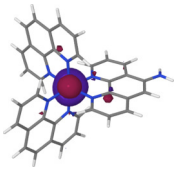
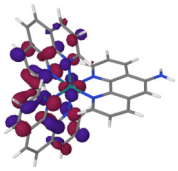
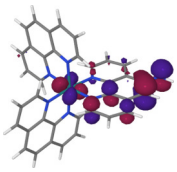
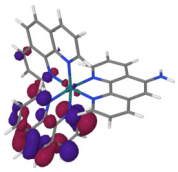
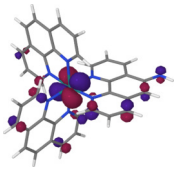
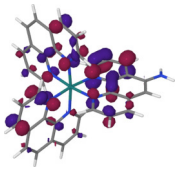
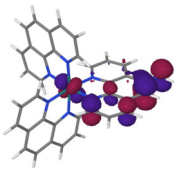
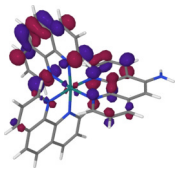
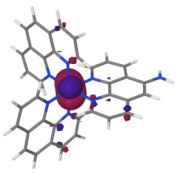
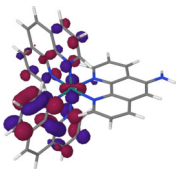


Figure S25: Absorption spectrum of $[Ru(phen)_2(phen\text{-}NH_2)]^{2+}$ obtained by convoluting the calculated oscillators strengths f with Gaussian having a full-with-at-half-maximum of 2000 cm^{-1} (SAOP/TZ2P results).

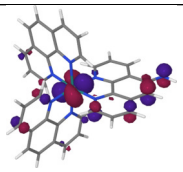
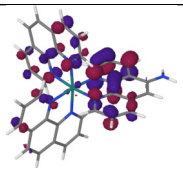
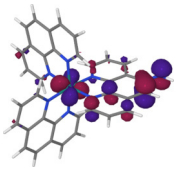
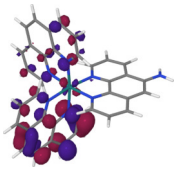
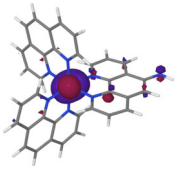
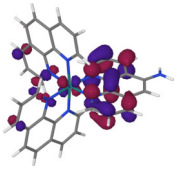
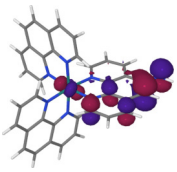
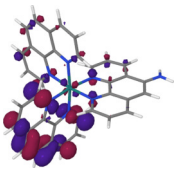
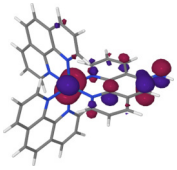
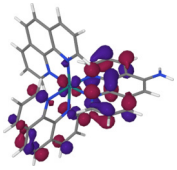
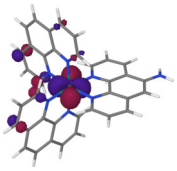
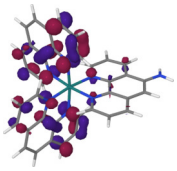
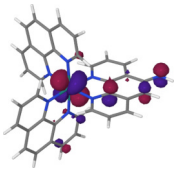
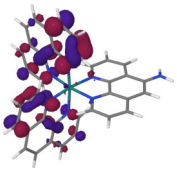
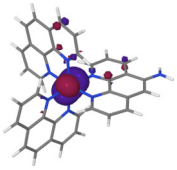
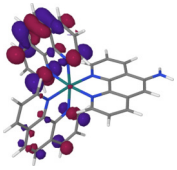
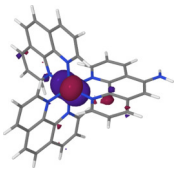
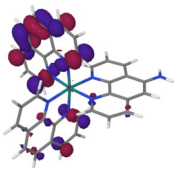
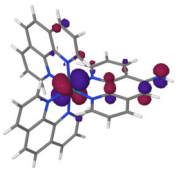
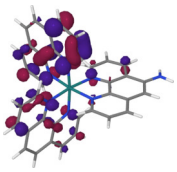
S8.3 Analysis of the electronic absorption spectrum

Table S2: Features of the $S_0 \rightarrow S_n$ electronic transition in $[Ru(phen)_2(phen\text{-}NH_2)]^{2+}$: transition wavelength λ, oscillator strength f, description in terms of natural transition orbitals (NTO) with the weights ω of NTO $\rightarrow$ NTO transitions (SAOP/TZ2P results)

n	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
1	609	0.004	99			
2	586	0.001	99			
3	578	0.000	99			
4	548	0.001	89			
5	546	0.000	51			
			28			
			21			
6	541	0.007	86			
7	537	0.002	52			

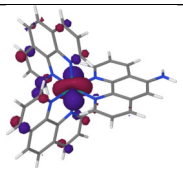
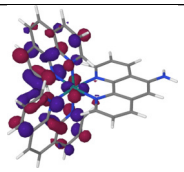
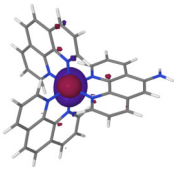
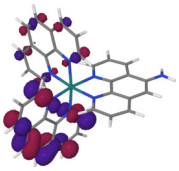
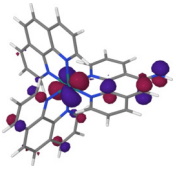
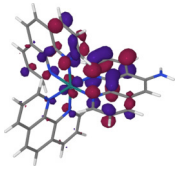
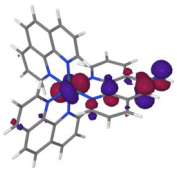
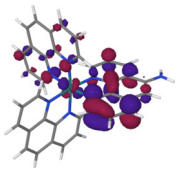
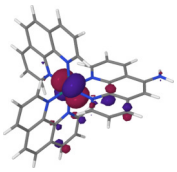
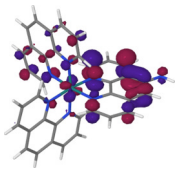
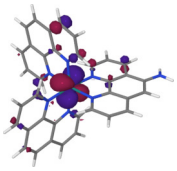
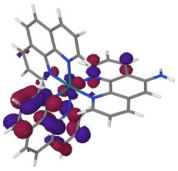
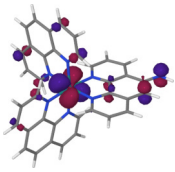
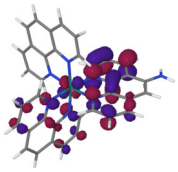
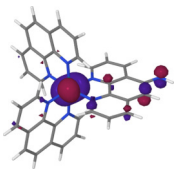
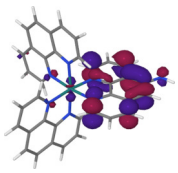
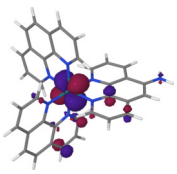
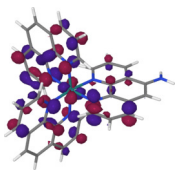
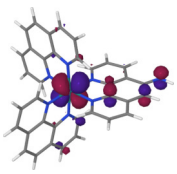
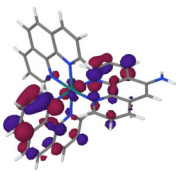
To be continued

Table S2: *continued*

n	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
			28			
			19			
8	534	0.018	63			
			26			
9	530	0.018	66			
			25			
10	525	0.004	52			
			46			
11	518	0.002	49			
			35			

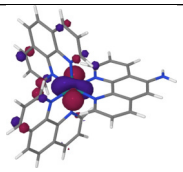
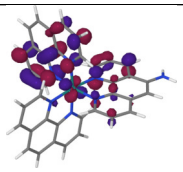
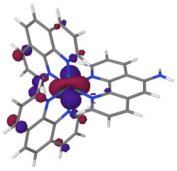
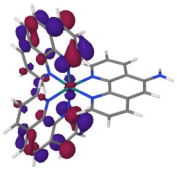
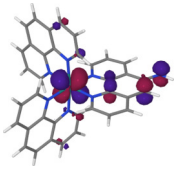
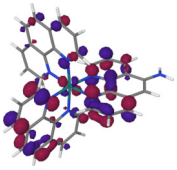
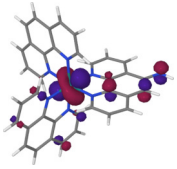
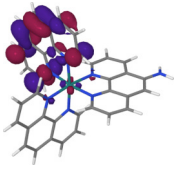
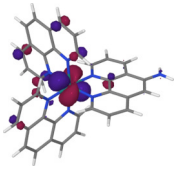
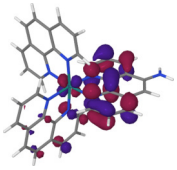
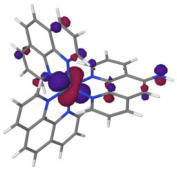
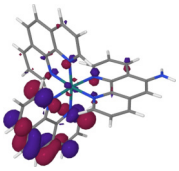
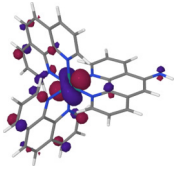
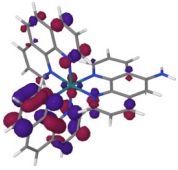
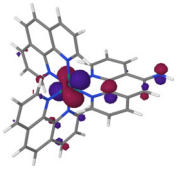
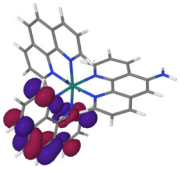
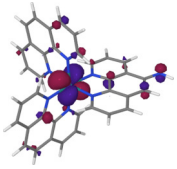
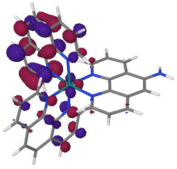
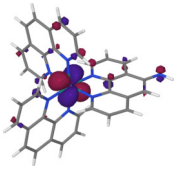
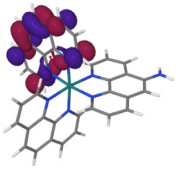
To be continued

Table S2: *continued*

n	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
			12			
12	512	0.015	83			
			11			
13	508	0.003	44			
			32			
			16			
14	485	0.001	51			
			29			
			17			
15	482	0.004	56			

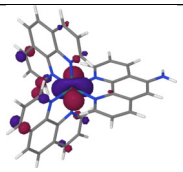
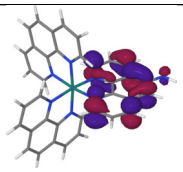
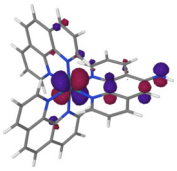
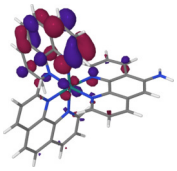
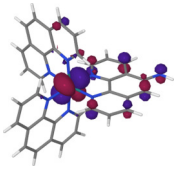
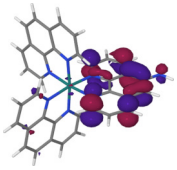
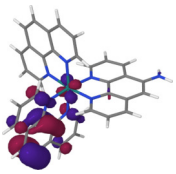
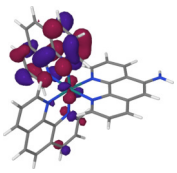
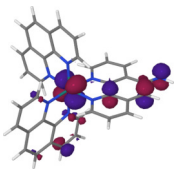
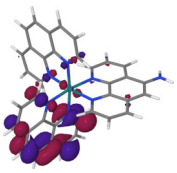
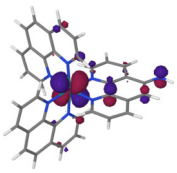
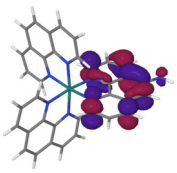
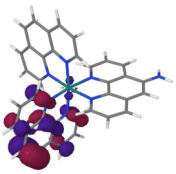
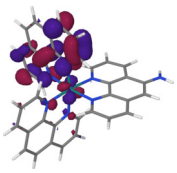
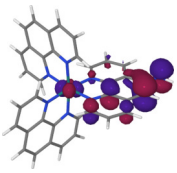
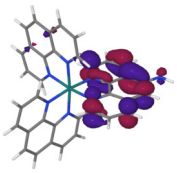
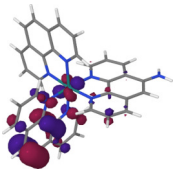
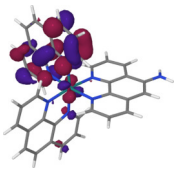
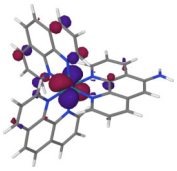
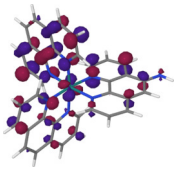
To be continued

Table S2: *continued*

n	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
			37			
16	478	0.001	72			
			21			
17	467	0.031	74			
			20			
18	466	0.031	68			
			23			
19	461	0.092	70			
			14			
20	459	0.105	87			

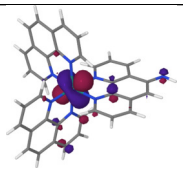
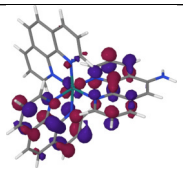
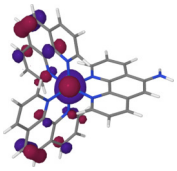
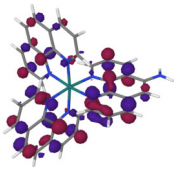
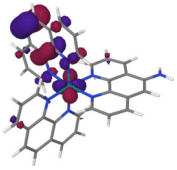
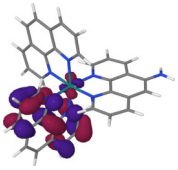
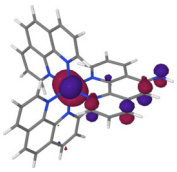
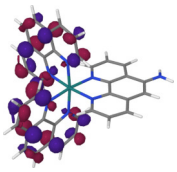
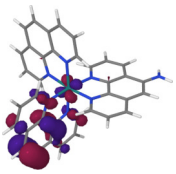
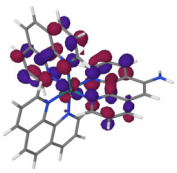
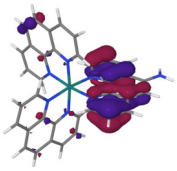
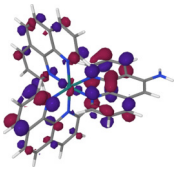
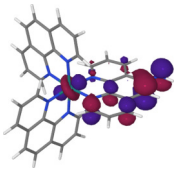
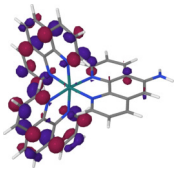
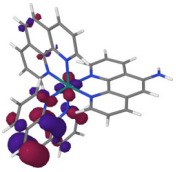
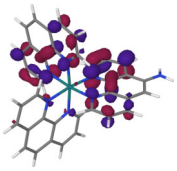
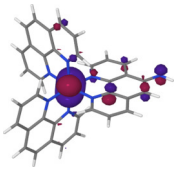
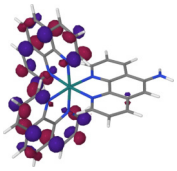
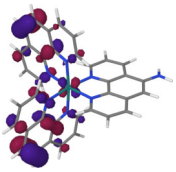
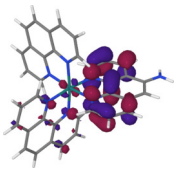
To be continued

Table S2: *continued*

n	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
21	452	0.031	87			
			10			
22	436	0.023	49			
			21			
			13			
23	420	0.038	76			
			13			
24	412	0.022	73			
			13			
25	382	0.001	39			

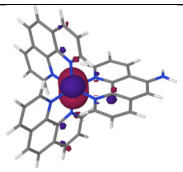
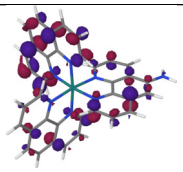
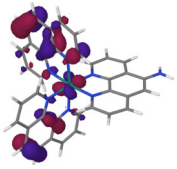
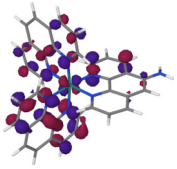
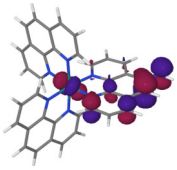
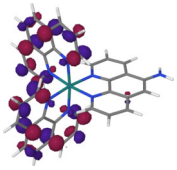
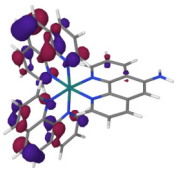
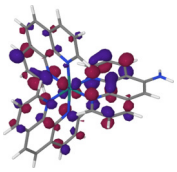
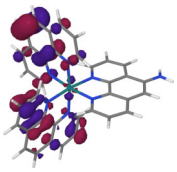
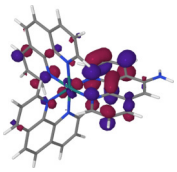
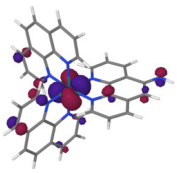
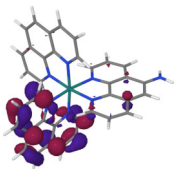
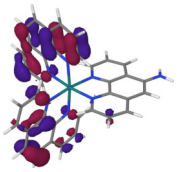
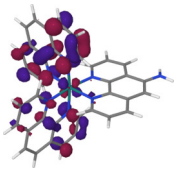
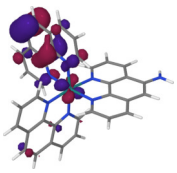
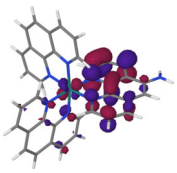
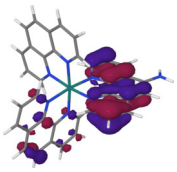
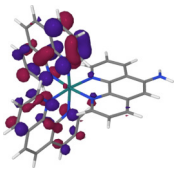
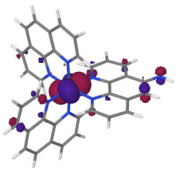
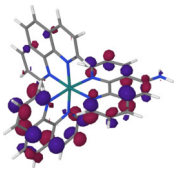
To be continued

Table S2: *continued*

n	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
			32			
			11			
26	378	0.001	52			
			22			
			14			
27	375	0.007	46			
			25			
28	369	0.002	61			
			24			
29	369	0.005	69			

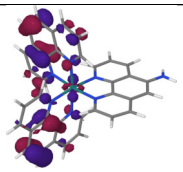
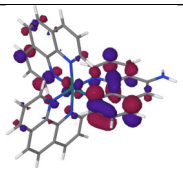
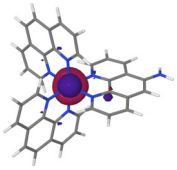
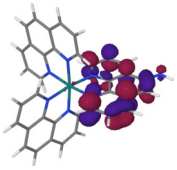
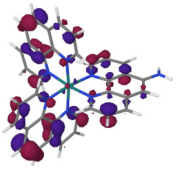
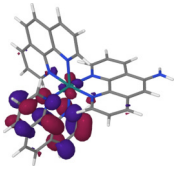
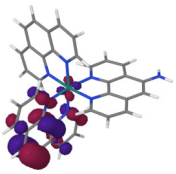
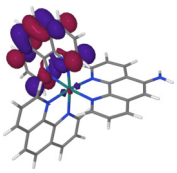
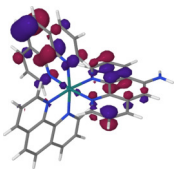
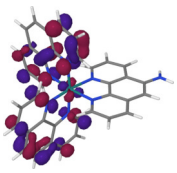
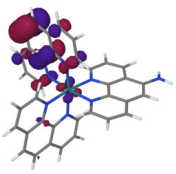
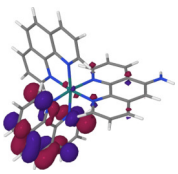
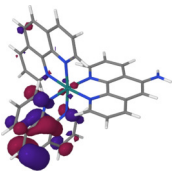
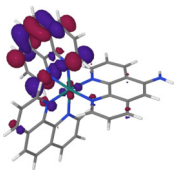
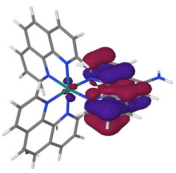
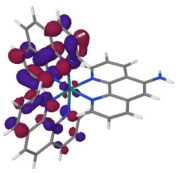
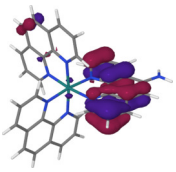
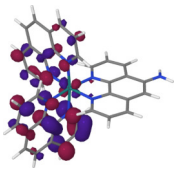
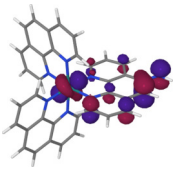
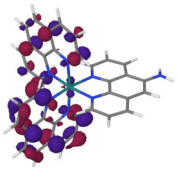
To be continued

Table S2: *continued*

n	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
			15			
			11			
30	367	0.004	70			
			17			
31	359	0.001	42			
			25			
			15			
32	356	0.001	48			
			18			
			16			

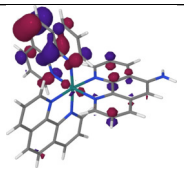
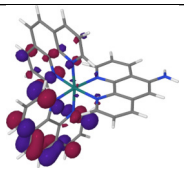
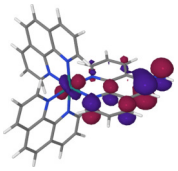
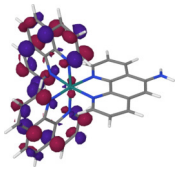
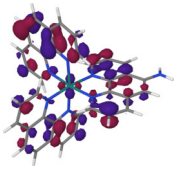
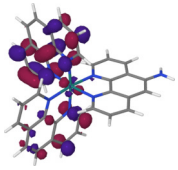
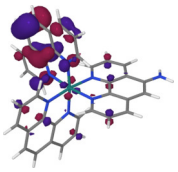
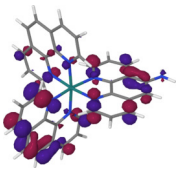
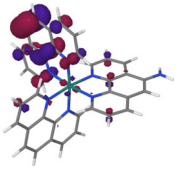
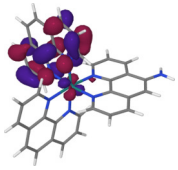
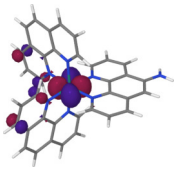
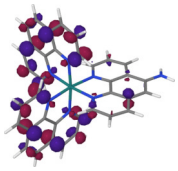
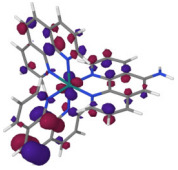
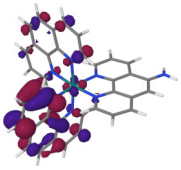
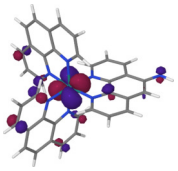
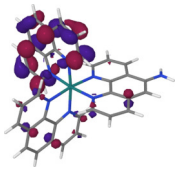
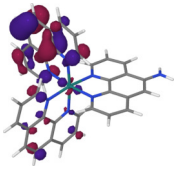
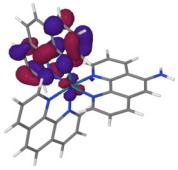
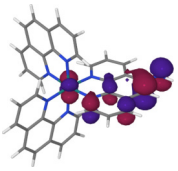
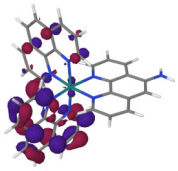
To be continued

Table S2: *continued*

n	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
33	356	0.003	54			
			11			
			10			
34	353	0.000	74			
			14			
35	351	0.001	65			
			15			
			11			
36	349	0.005	52			
			20			

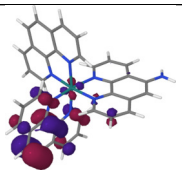
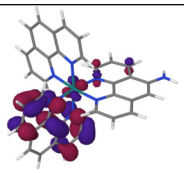
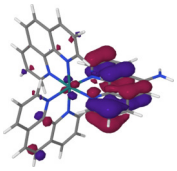
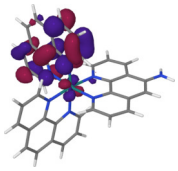
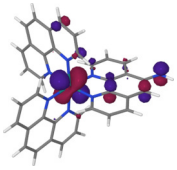
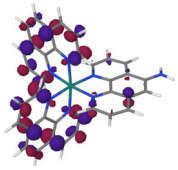
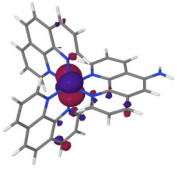
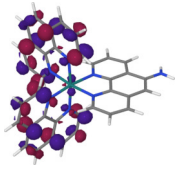
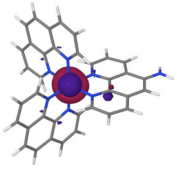
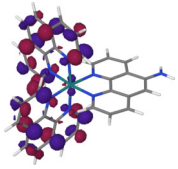
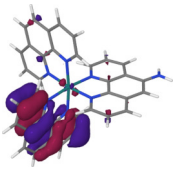
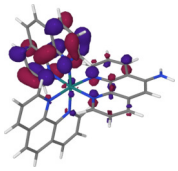
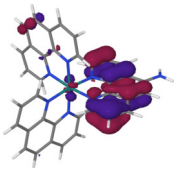
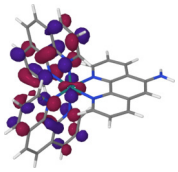
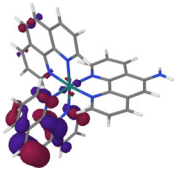
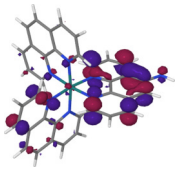
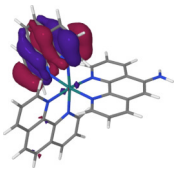
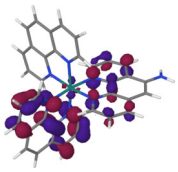
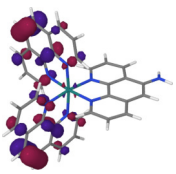
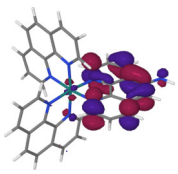
To be continued

Table S2: *continued*

n	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
37	347	0.012	16			
			45			
			19			
			15			
38	344	0.008	56			
			12			
			10			
39	344	0.003	39			
			28			
			20			

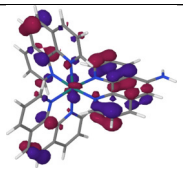
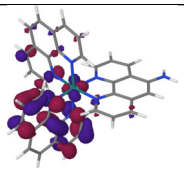
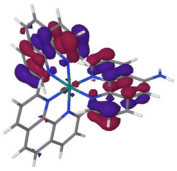
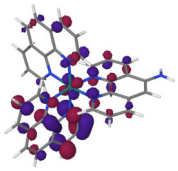
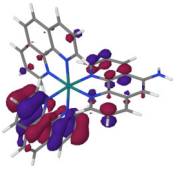
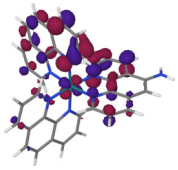
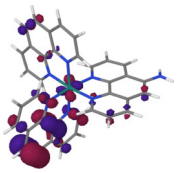
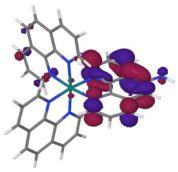
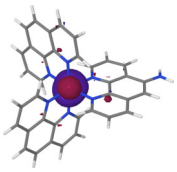
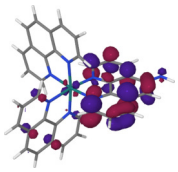
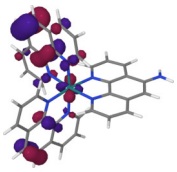
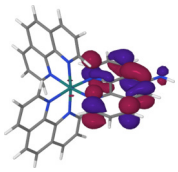
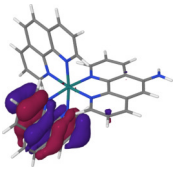
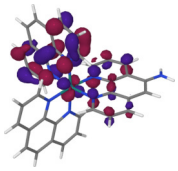
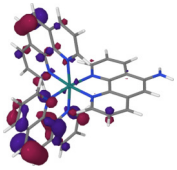
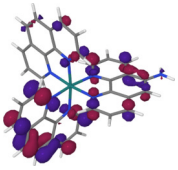
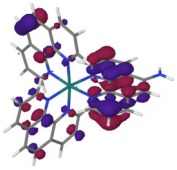
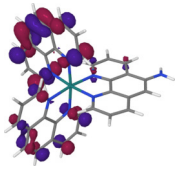
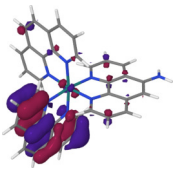
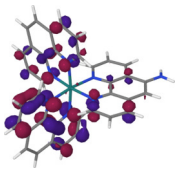
To be continued

Table S2: *continued*

n	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
40	343	0.001	51			
			18			
41	342	0.000	80			
			10			
42	340	0.001	66			
			24			
43	339	0.001	62			
			22			
44	336	0.003	86			
45	334	0.000	61			

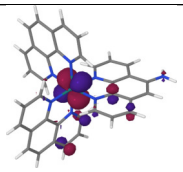
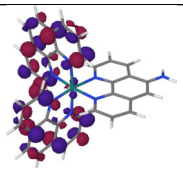
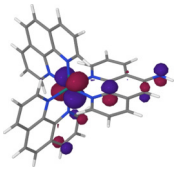
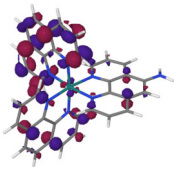
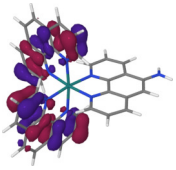
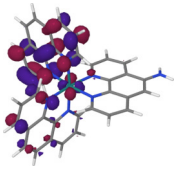
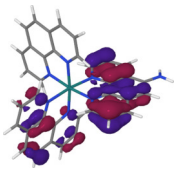
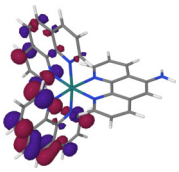
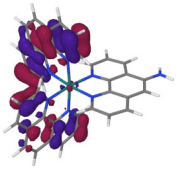
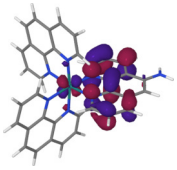
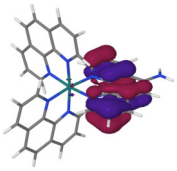
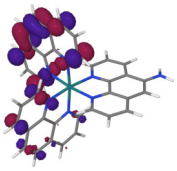
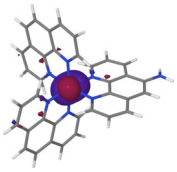
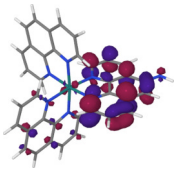
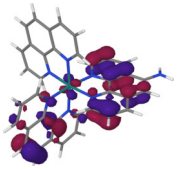
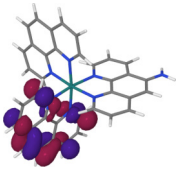
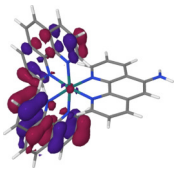
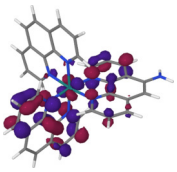
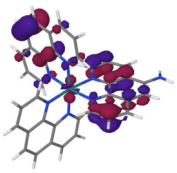
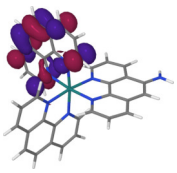
To be continued

Table S2: *continued*

n	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
			21			
46	333	0.003	35			
			31			
			16			
47	332	0.003	47			
			30			
			14			
48	331	0.001	38			
			26			
			12			

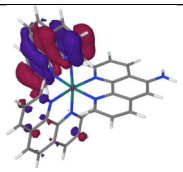
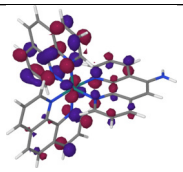
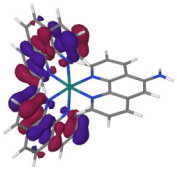
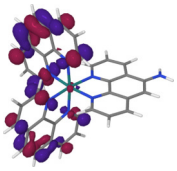
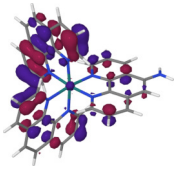
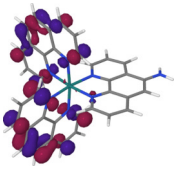
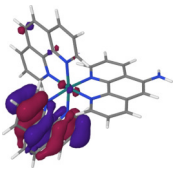
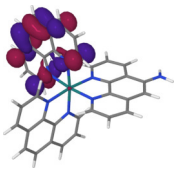
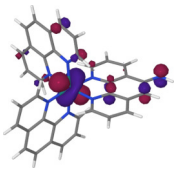
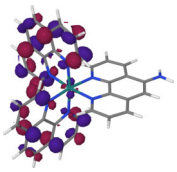
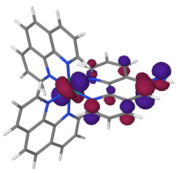
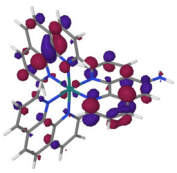
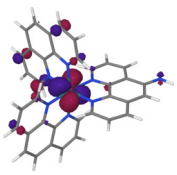
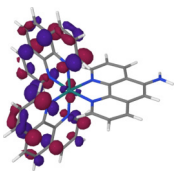
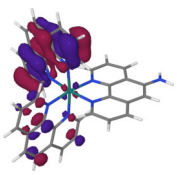
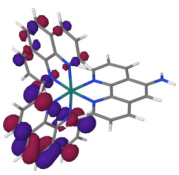
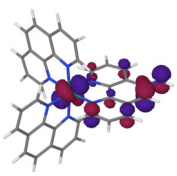
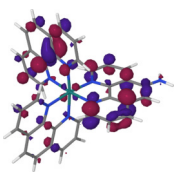
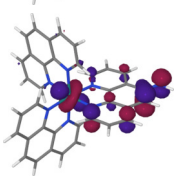
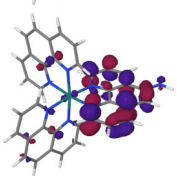
To be continued

Table S2: *continued*

n	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
			12			
49	330	0.002	39			
			30			
			14			
50	326	0.002	66			
			18			
			10			
51	325	0.003	67			
			14			
52	323	0.002	64			

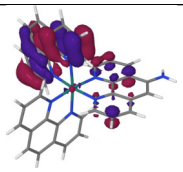
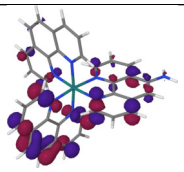
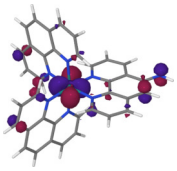
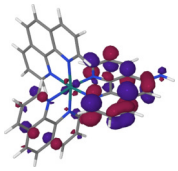
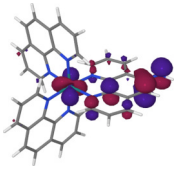
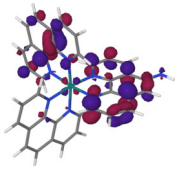
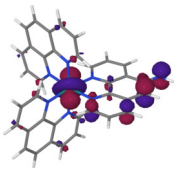
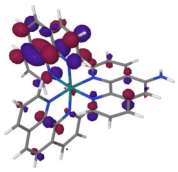
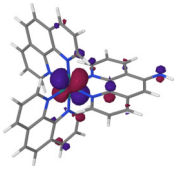
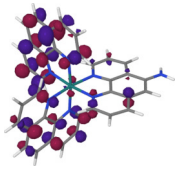
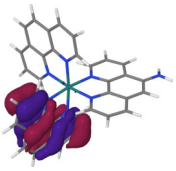
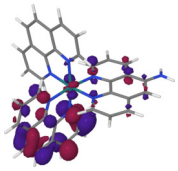
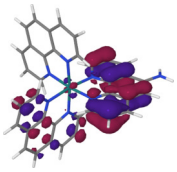
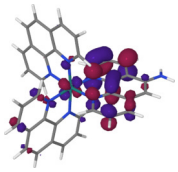
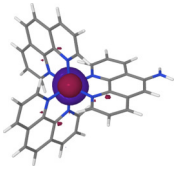
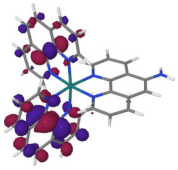
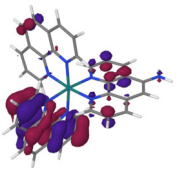
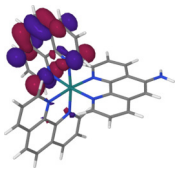
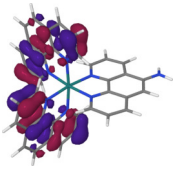
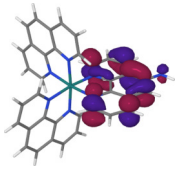
To be continued

Table S2: *continued*

n	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
			19			
53	322	0.007	50			
			27			
54	321	0.007	52			
			20			
			14			
55	320	0.012	36			
			34			
			14			
56	317	0.010	50			

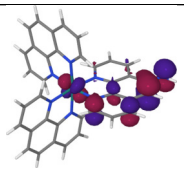
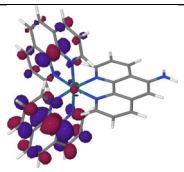
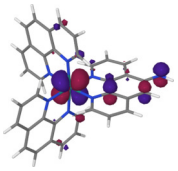
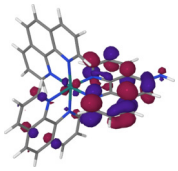
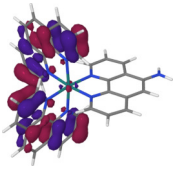
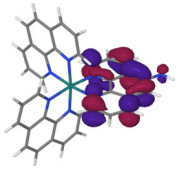
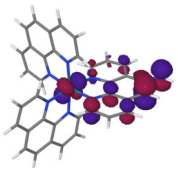
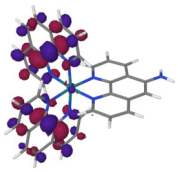
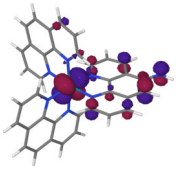
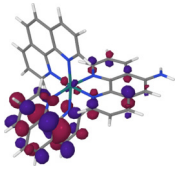
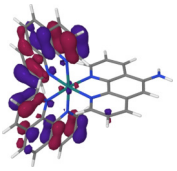
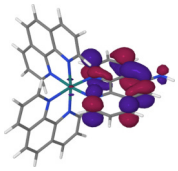
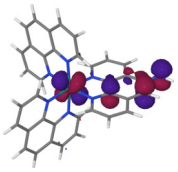
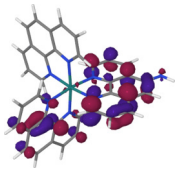
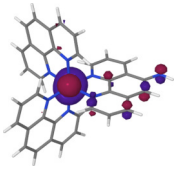
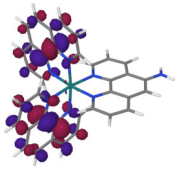
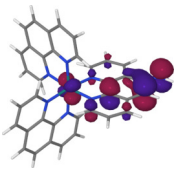
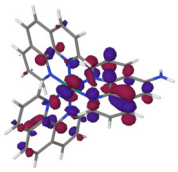
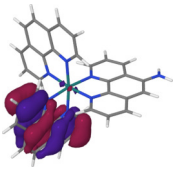
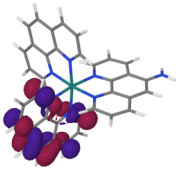
To be continued

Table S2: *continued*

n	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
			21			
57	313	0.007	76			
58	309	0.003	40			
			18			
			14			
			11			
59	307	0.000	49			
			19			
			11			
60	305	0.002	92			

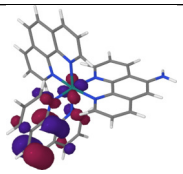
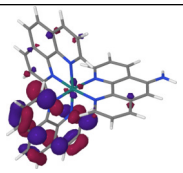
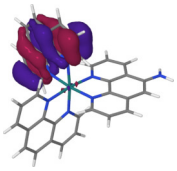
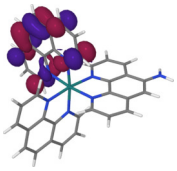
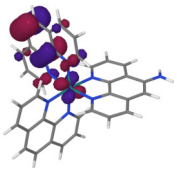
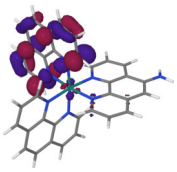
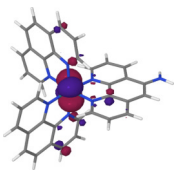
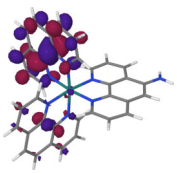
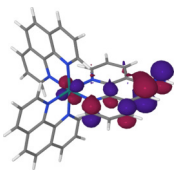
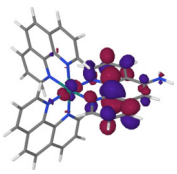
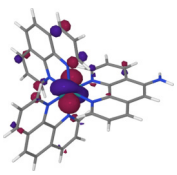
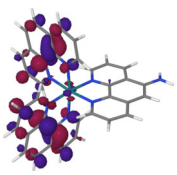
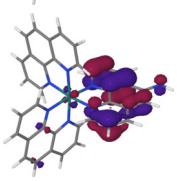
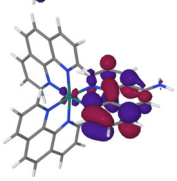
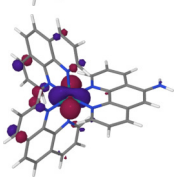
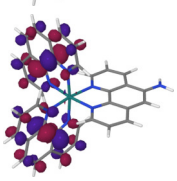
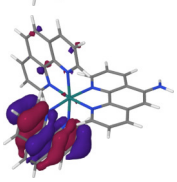
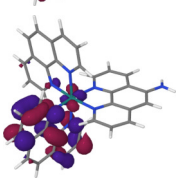
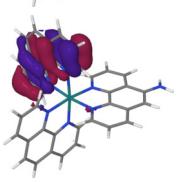
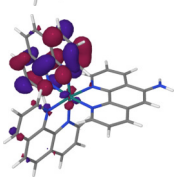
To be continued

Table S2: *continued*

n	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
61	305	0.002	72			
			16			
62	302	0.023	54			
			29			
63	298	0.009	32			
			26			
			22			
64	297	0.121	47			
			13			
65	295	0.013	58			

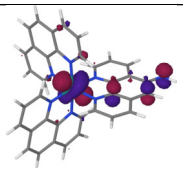
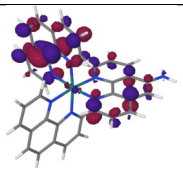
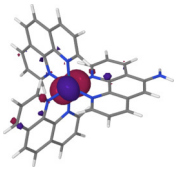
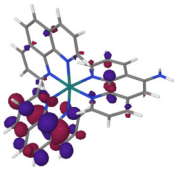
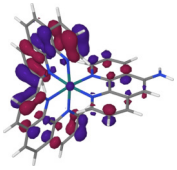
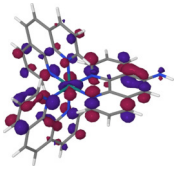
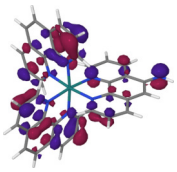
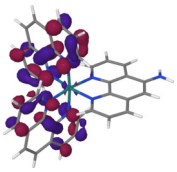
To be continued

Table S2: *continued*

n	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
			13			
66	295	0.068	62			
			15			
67	292	0.023	62			
68	288	0.023	38			
			17			
			11			
69	287	0.026	38			
			15			
			12			

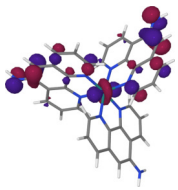
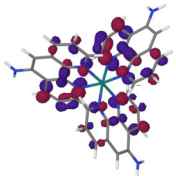
To be continued

Table S2: *continued*

n	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
70	286	0.013	24			
			19			
			15			
			13			

S9 Computational results: $[Ru(phen\text{-}NH_2)_3]^{2+}$

S9.1 HOMO-LUMO gap

HOMO	LUMO
	
$\varepsilon_{HOMO} = -14.147$ eV	$\varepsilon_{LUMO} = -12.108$ eV
$\Delta\varepsilon = 2.039$ eV	

S9.2 Calculated absorption spectrum

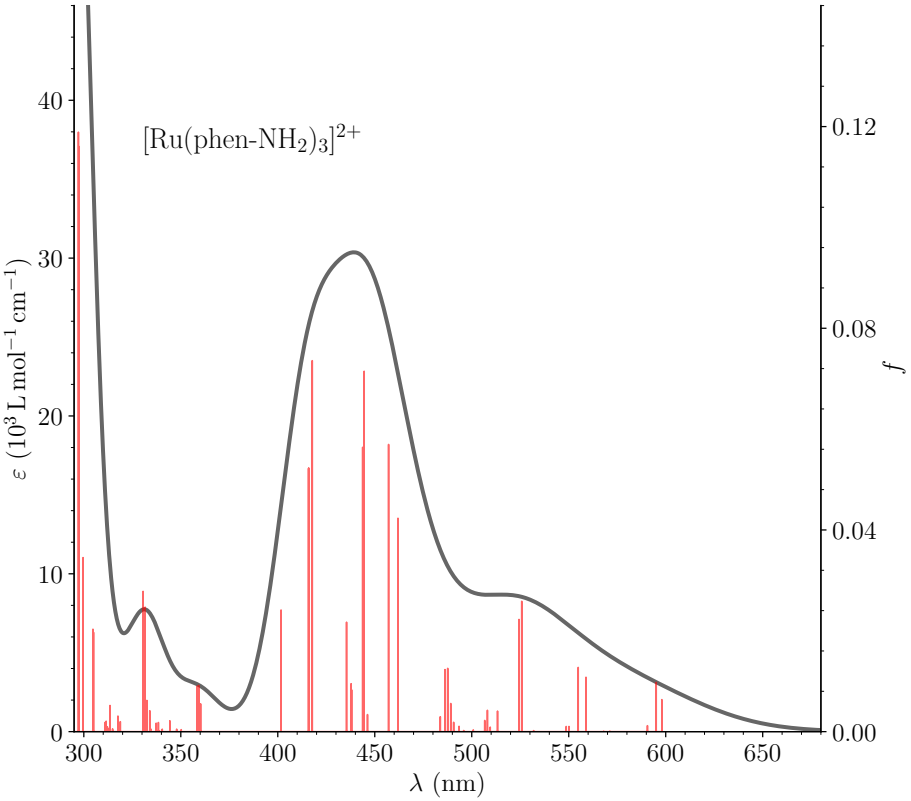
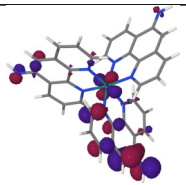
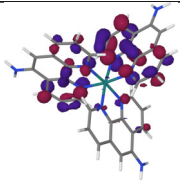
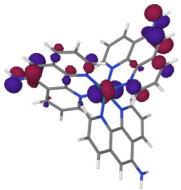
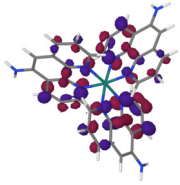
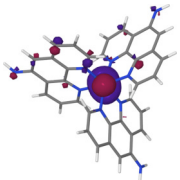
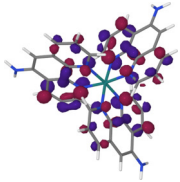
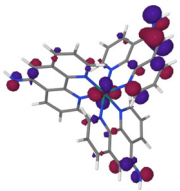
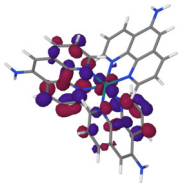
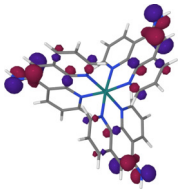
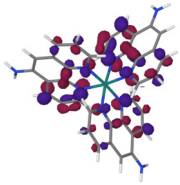
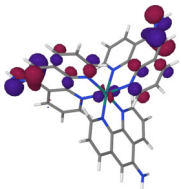
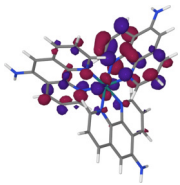
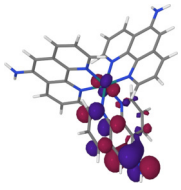
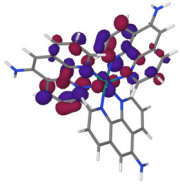
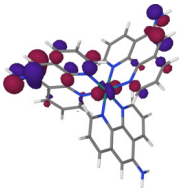
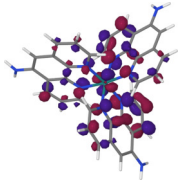


Figure S26: Absorption spectrum of $[Ru(phen\text{-}NH_2)_3]^{2+}$ obtained by convoluting the calculated oscillators strengths f with Gaussian having a full-with-at-half-maximum of 2000 cm^{-1} (SAOP/TZ2P results).

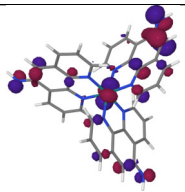
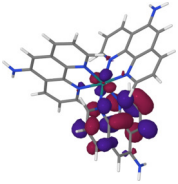
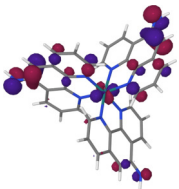
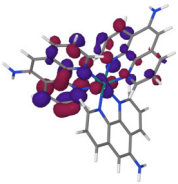
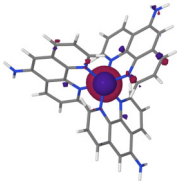
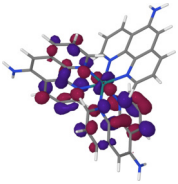
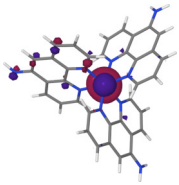
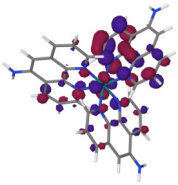
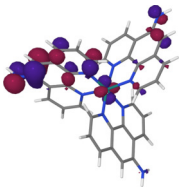
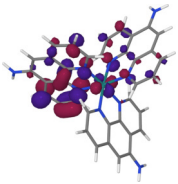
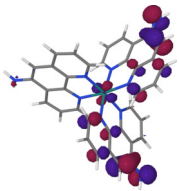
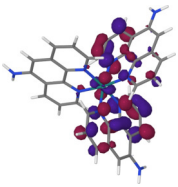
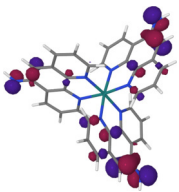
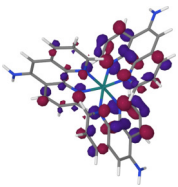
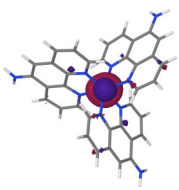
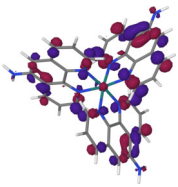
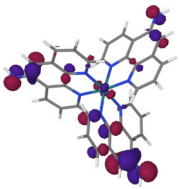
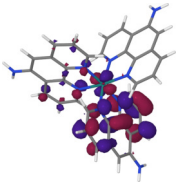
S9.3 Analysis of the electronic absorption spectrum

Table S3: Features of the $S_0 \rightarrow S_n$ electronic transition in $[Ru(phen\text{-}NH_2)_3]^{2+}$: transition wavelength λ, oscillator strength f, description in terms of natural transition orbitals (NTO) with the weights ω of NTO $\rightarrow$ NTO transitions (SAOP/TZ2P results)

n	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
1	598	0.006	95			
2	595	0.010	92			
3	591	0.001	98			
4	571	0.000	53			
			45			
5	568	0.000	71			
			22			
6	559	0.011	54			
			43			

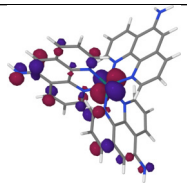
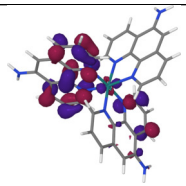
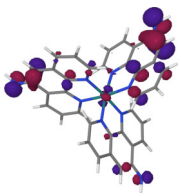
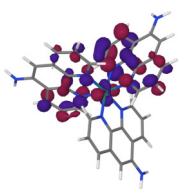
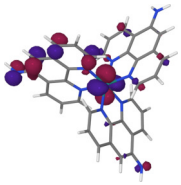
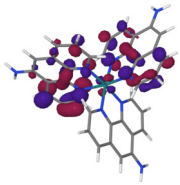
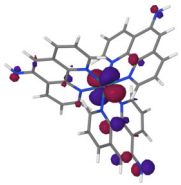
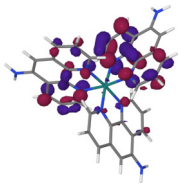
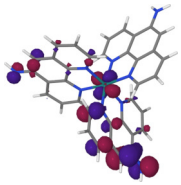
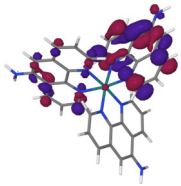
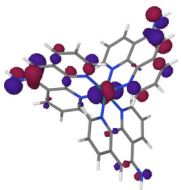
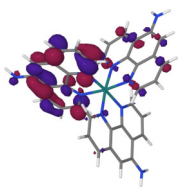
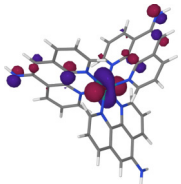
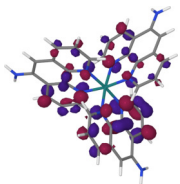
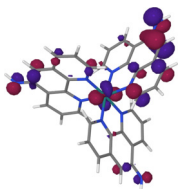
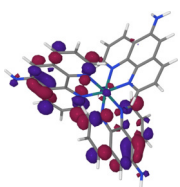
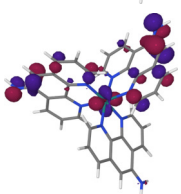
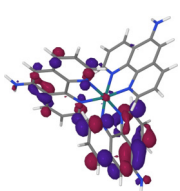
To be continued

Table S3: *continued*

n	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
7	555	0.013	66			
			33			
8	550	0.001	95			
9	549	0.001	94			
10	532	0.000	34			
			31			
			21			
			12			
11	526	0.026	81			

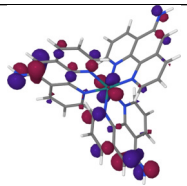
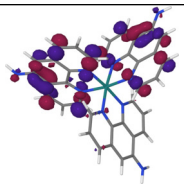
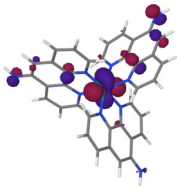
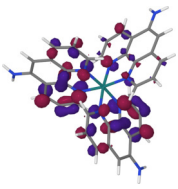
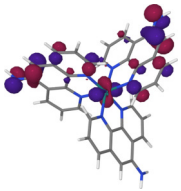
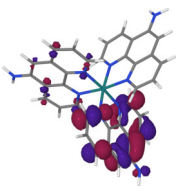
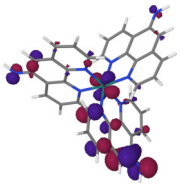
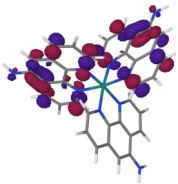
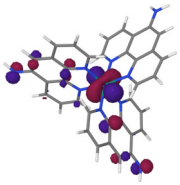
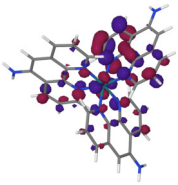
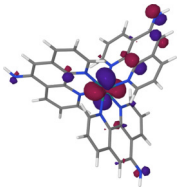
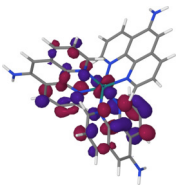
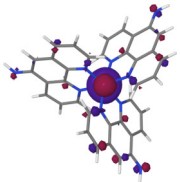
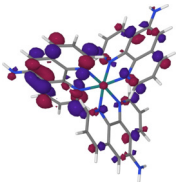
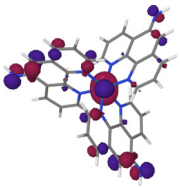
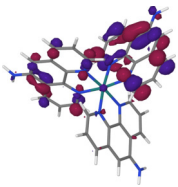
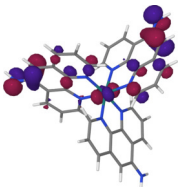
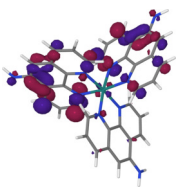
To be continued

Table S3: *continued*

n	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
			10			
12	524	0.022	80			
			12			
13	513	0.004	85			
14	510	0.001	84			
			12			
15	508	0.004	66			
			18			
16	507	0.002	57			

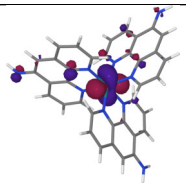
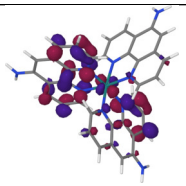
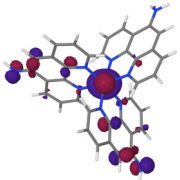
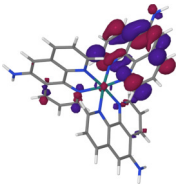
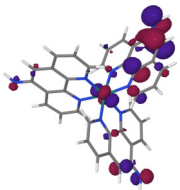
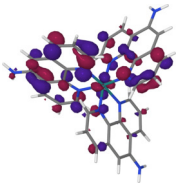
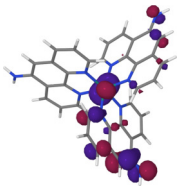
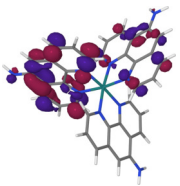
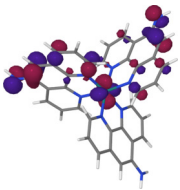
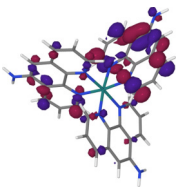
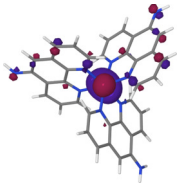
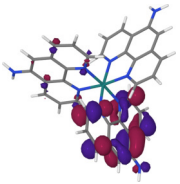
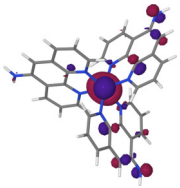
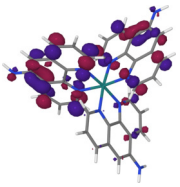
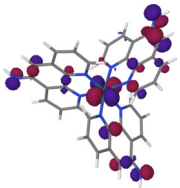
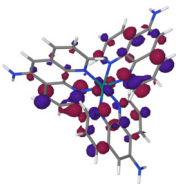
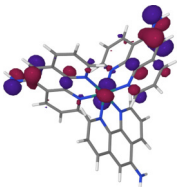
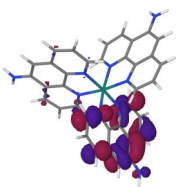
To be continued

Table S3: *continued*

n	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
			22			
			15			
17	501	0.000	55			
			40			
18	496	0.000	43			
			40			
			12			
19	493	0.001	54			
			21			

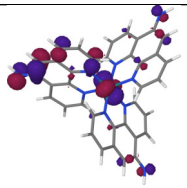
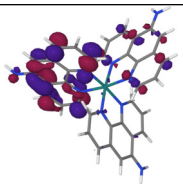
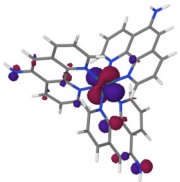
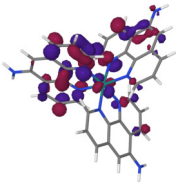
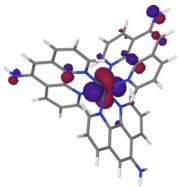
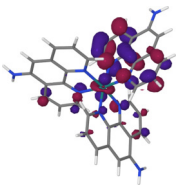
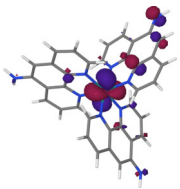
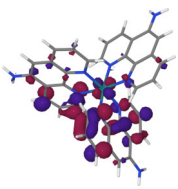
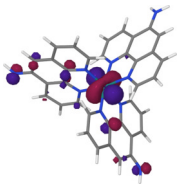
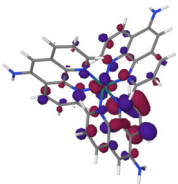
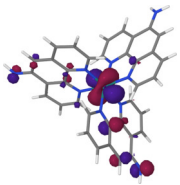
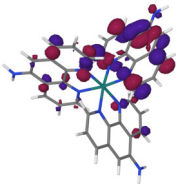
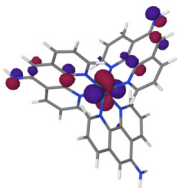
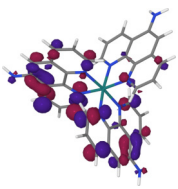
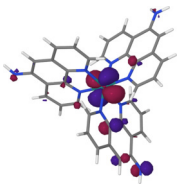
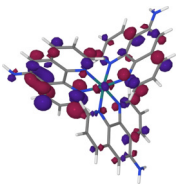
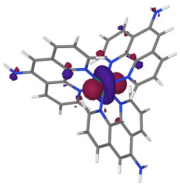
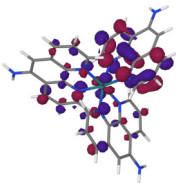
To be continued

Table S3: *continued*

n	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
			14			
20	491	0.002	69			
			17			
21	489	0.006	68			
			24			
22	488	0.013	80			
23	486	0.012	73			
			10			
24	484	0.003	84			

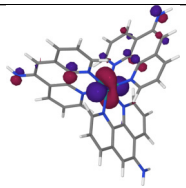
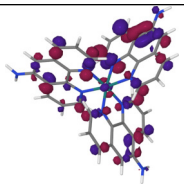
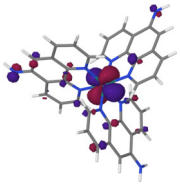
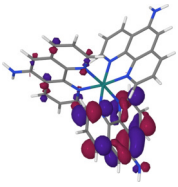
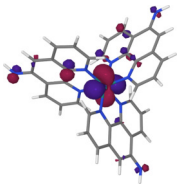
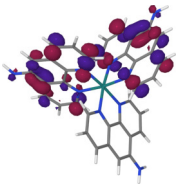
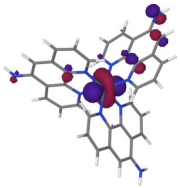
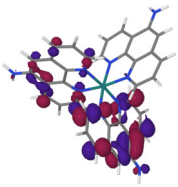
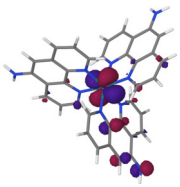
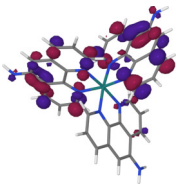
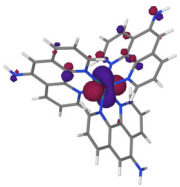
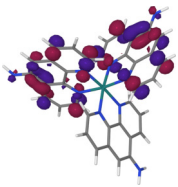
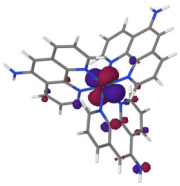
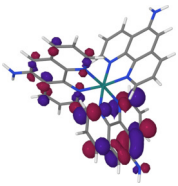
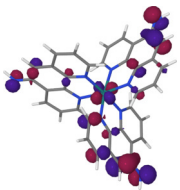
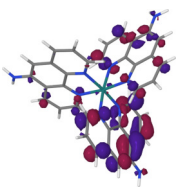
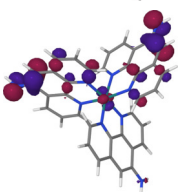
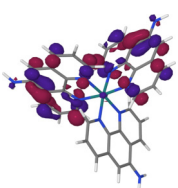
To be continued

Table S3: *continued*

n	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
			13			
25	462	0.042	49			
			41			
26	457	0.057	48			
			41			
27	446	0.003	61			
			36			
28	445	0.071	81			
			12			

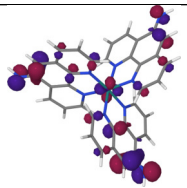
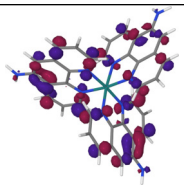
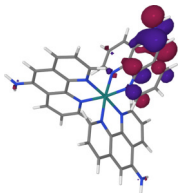
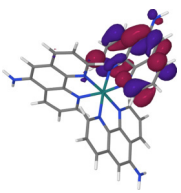
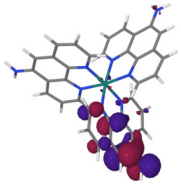
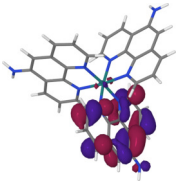
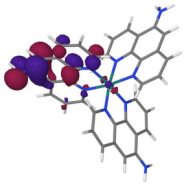
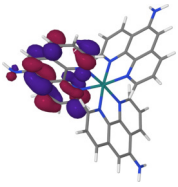
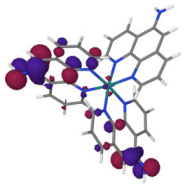
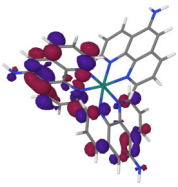
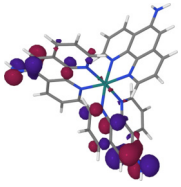
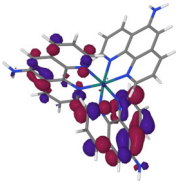
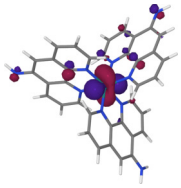
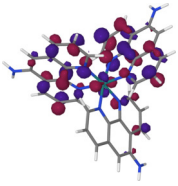
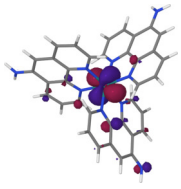
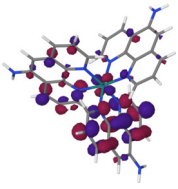
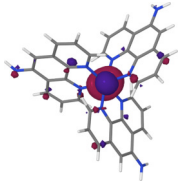
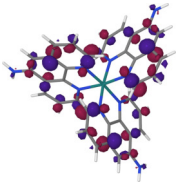
To be continued

Table S3: *continued*

n	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
29	444	0.056	85			
30	438	0.008	73			
			23			
31	438	0.009	58			
			38			
32	435	0.022	69			
			25			
33	418	0.074	32			
			28			

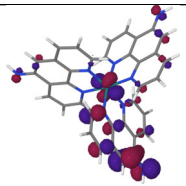
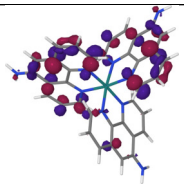
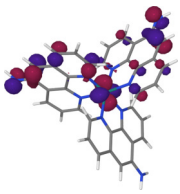
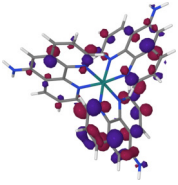
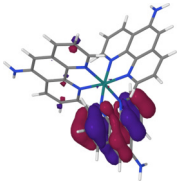
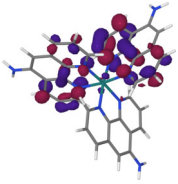
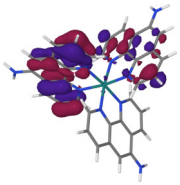
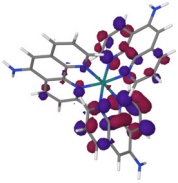
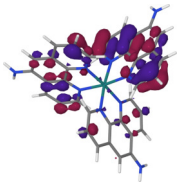
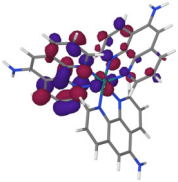
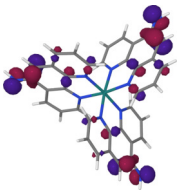
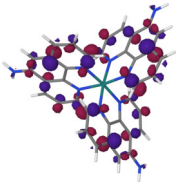
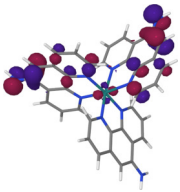
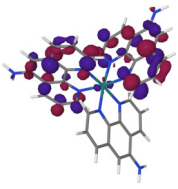
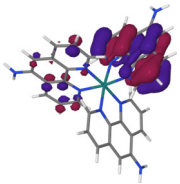
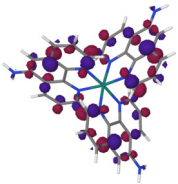
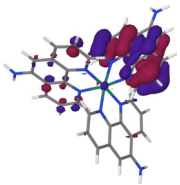
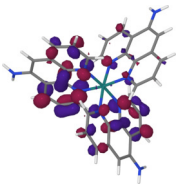
To be continued

Table S3: *continued*

n	λ (nm)	f	NTO			
			ω (%)	occ.	→	virt.
			25			
34	416	0.052	54			
			19			
			17			
35	416	0.052	53			
			36			
36	402	0.024	37			
			33			
37	360	0.006	93			

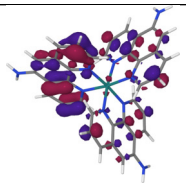
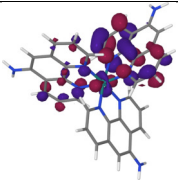
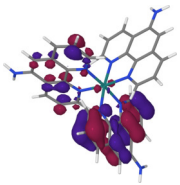
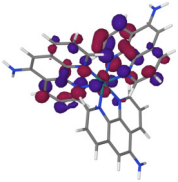
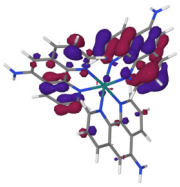
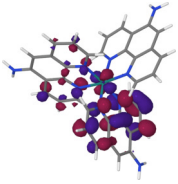
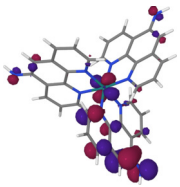
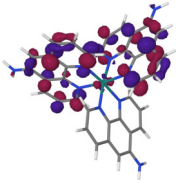
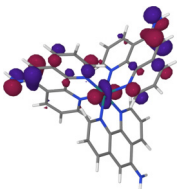
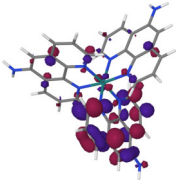
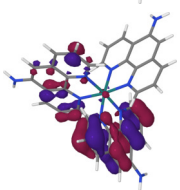
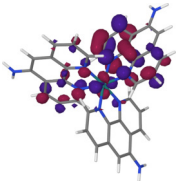
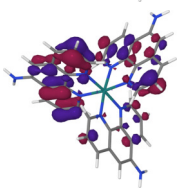
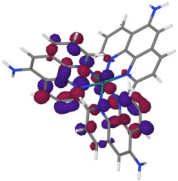
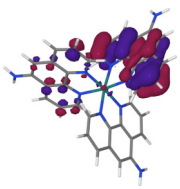
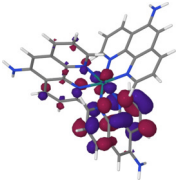
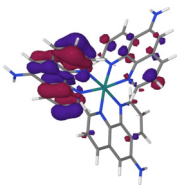
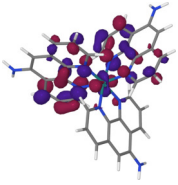
To be continued

Table S3: *continued*

n	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
38	359	0.009	91			
39	358	0.009	90			
40	350	0.000	92			
41	348	0.000	73			
			16			
42	348	0.001	69			
			12			
			11			
43	344	0.002	65			

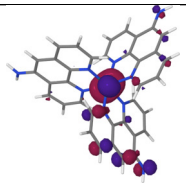
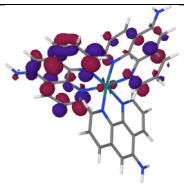
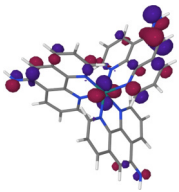
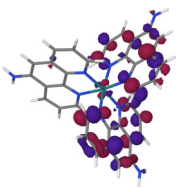
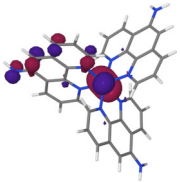
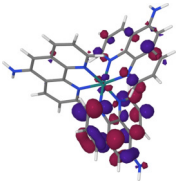
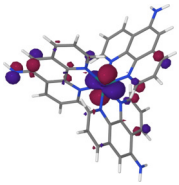
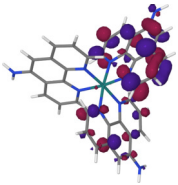
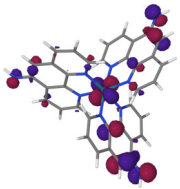
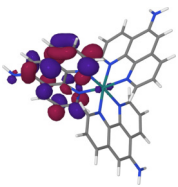
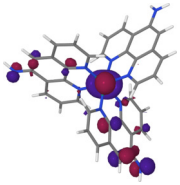
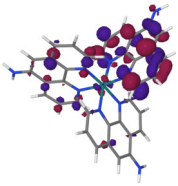
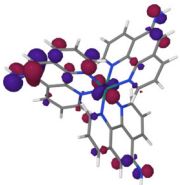
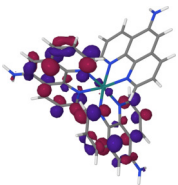
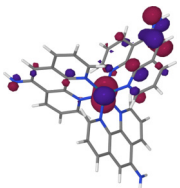
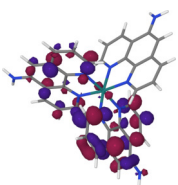
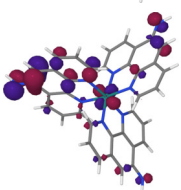
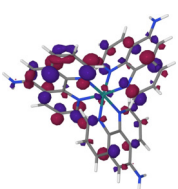
To be continued

Table S3: *continued*

n	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
			26			
44	340	0.001	53			
			41			
45	339	0.000	58			
			39			
46	338	0.002	63			
			35			
47	337	0.002	80			
			17			

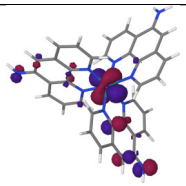
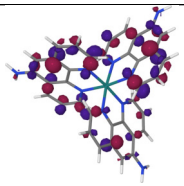
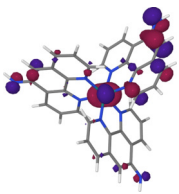
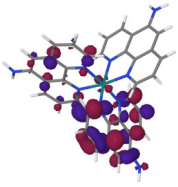
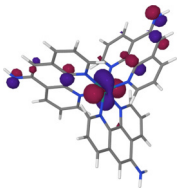
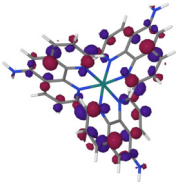
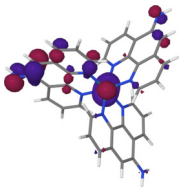
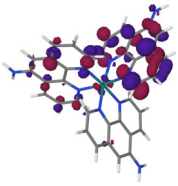
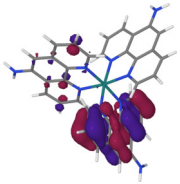
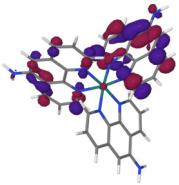
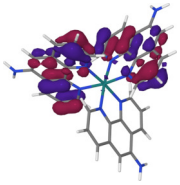
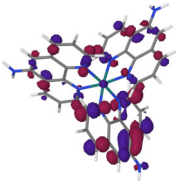
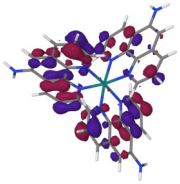
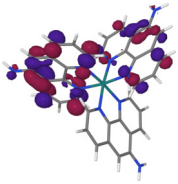
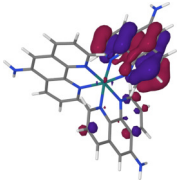
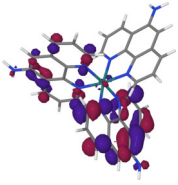
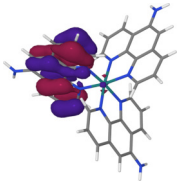
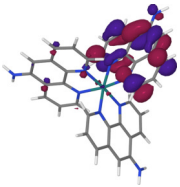
To be continued

Table S3: *continued*

n	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
48	336	0.000	71			
			20			
49	335	0.000	73			
			14			
			11			
50	334	0.004	76			
			16			
51	332	0.006	73			
			17			

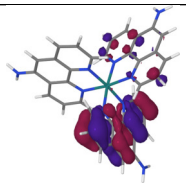
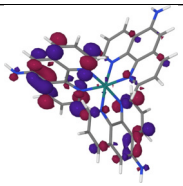
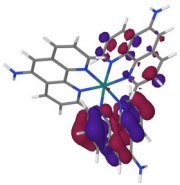
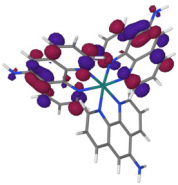
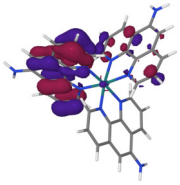
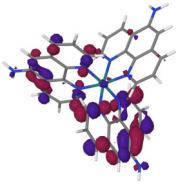
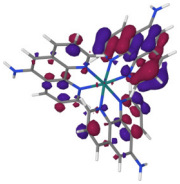
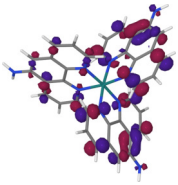
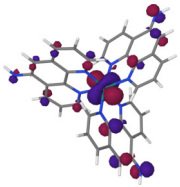
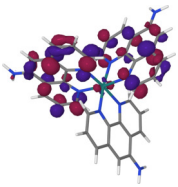
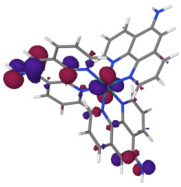
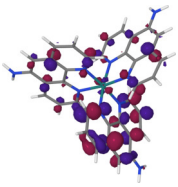
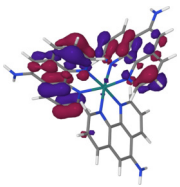
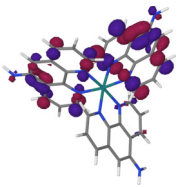
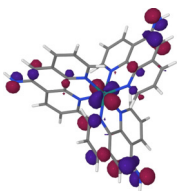
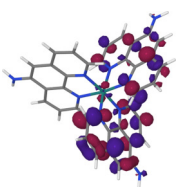
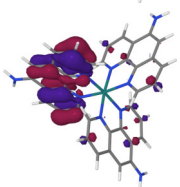
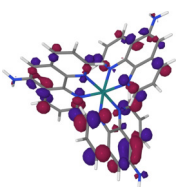
To be continued

Table S3: *continued*

n	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
52	332	0.025	74			
			18			
53	331	0.028	82			
			11			
54	319	0.002	92			
55	318	0.003	74			
			22			
56	315	0.000	47			
			30			

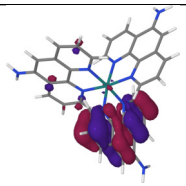
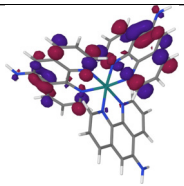
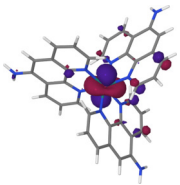
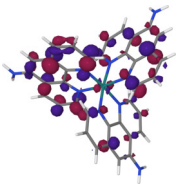
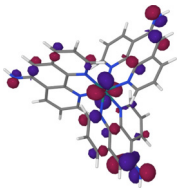
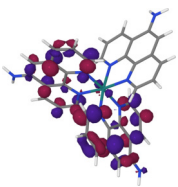
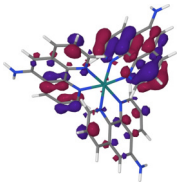
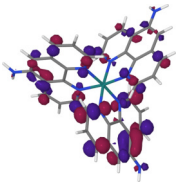
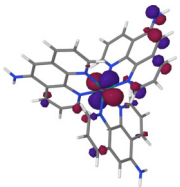
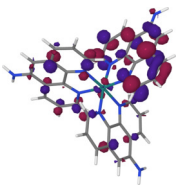
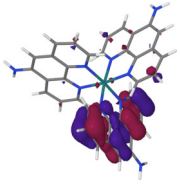
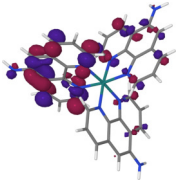
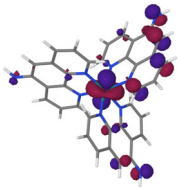
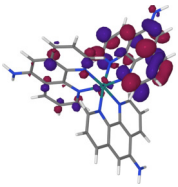
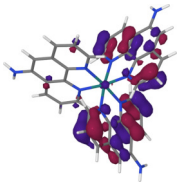
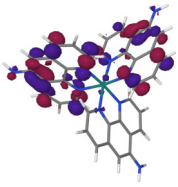
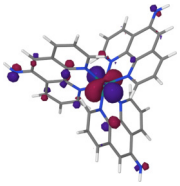
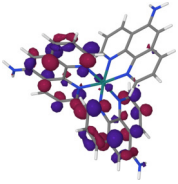
To be continued

Table S3: *continued*

n	λ (nm)	f	NTO			
			ω (%)	occ.	→	virt.
			13			
57	315	0.001	48			
			29			
			18			
58	313	0.005	44			
			22			
			19			
59	313	0.001	32			
			27			

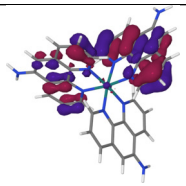
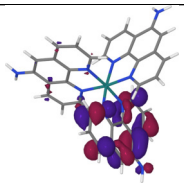
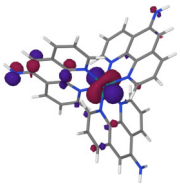
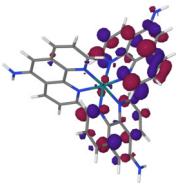
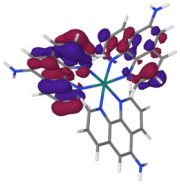
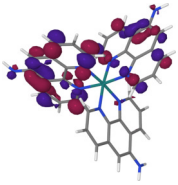
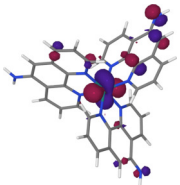
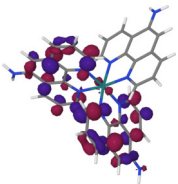
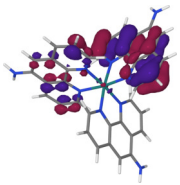
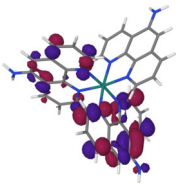
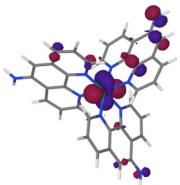
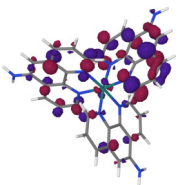
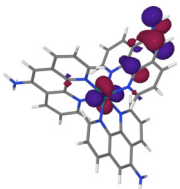
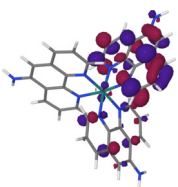
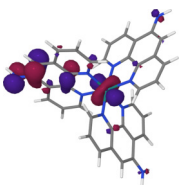
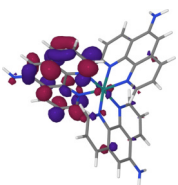
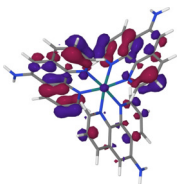
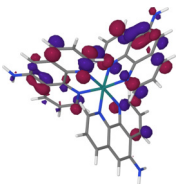
To be continued

Table S3: *continued*

n	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
			19			
			12			
60	313	0.000	41			
			21			
			17			
			14			
61	312	0.001	38			
			36			
			11			

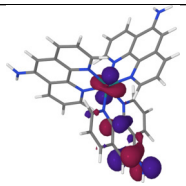
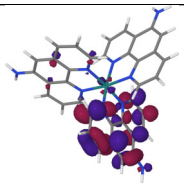
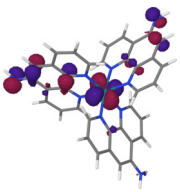
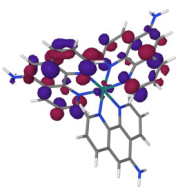
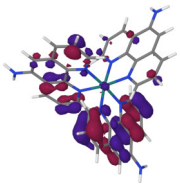
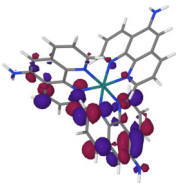
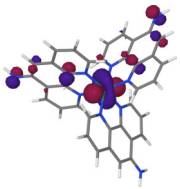
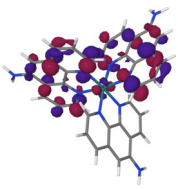
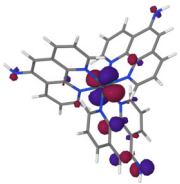
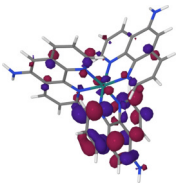
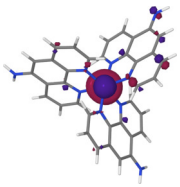
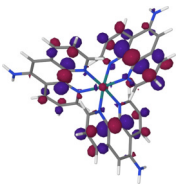
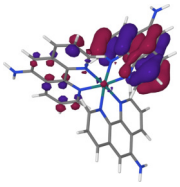
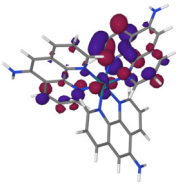
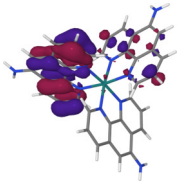
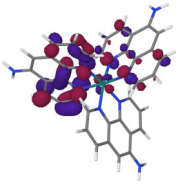
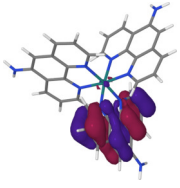
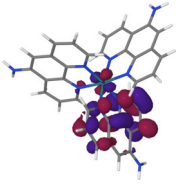
To be continued

Table S3: *continued*

n	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
62	311	0.002	55			
			19			
			16			
63	311	0.002	41			
			29			
			19			
64	305	0.020	41			
			33			
			15			

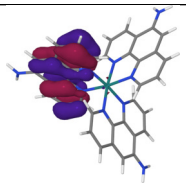
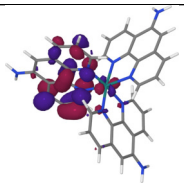
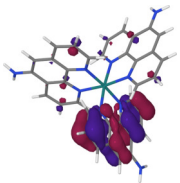
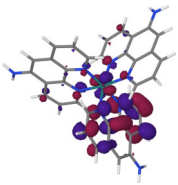
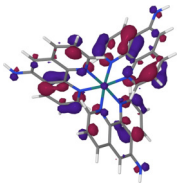
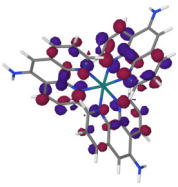
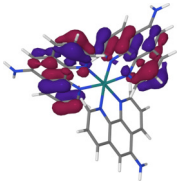
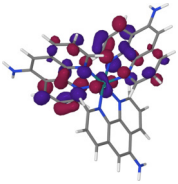
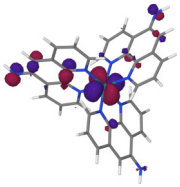
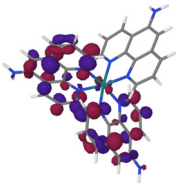
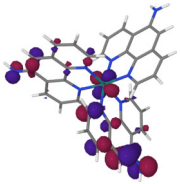
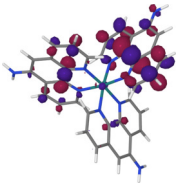
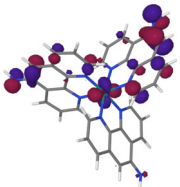
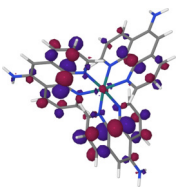
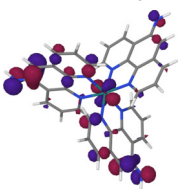
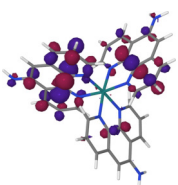
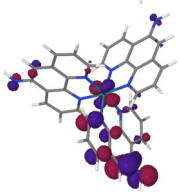
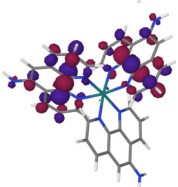
To be continued

Table S3: *continued*

n	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
65	305	0.020	44			
			28			
			16			
66	300	0.035	30			
			30			
			12			
67	297	0.116	42			
			23			
68	297	0.119	42			

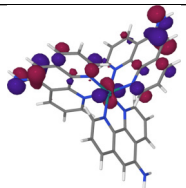
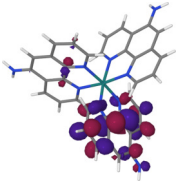
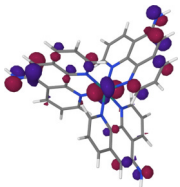
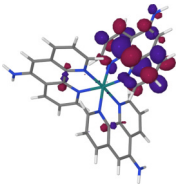
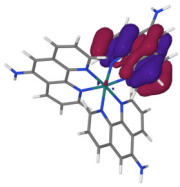
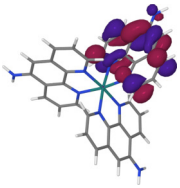
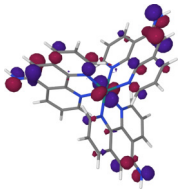
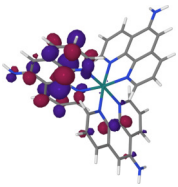
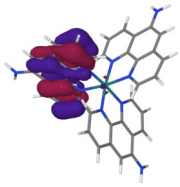
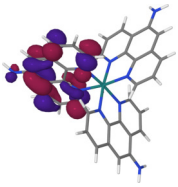
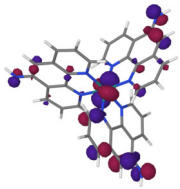
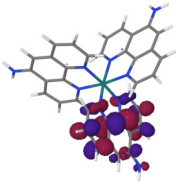
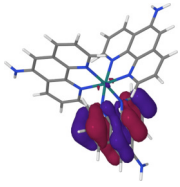
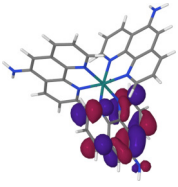
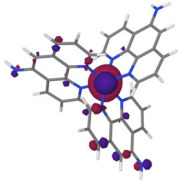
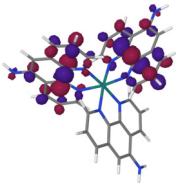
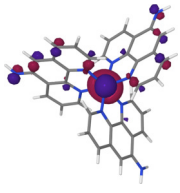
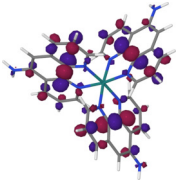
To be continued

Table S3: *continued*

n	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
			18			
69	294	0.256	20			
			18			
			18			
			10			
70	293	0.002	92			
71	292	0.002	85			
			11			
72	290	0.000	56			

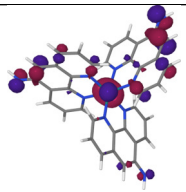
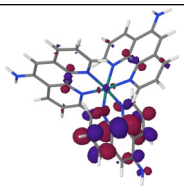
To be continued

Table S3: *continued*

n	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
			36			
73	289	0.003	77			
			11			
74	288	0.008	72			
			13			
75	287	0.007	70			
			19			
76	286	0.004	86			
77	285	0.003	76			

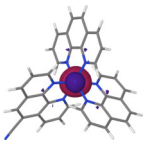
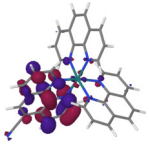
To be continued

Table S3: *continued*

n	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
78	285	0.003	69			

S10 Computational results: $[Ru(phen)_2(phen\text{-}CN)]^{2+}$

S10.1 HOMO-LUMO gap

HOMO	LUMO
	
$\varepsilon_{HOMO} = -14.811$ eV	$\varepsilon_{LUMO} = -12.717$ eV
$\Delta\varepsilon = 2.094$ eV	

S10.2 Calculated absorption spectrum

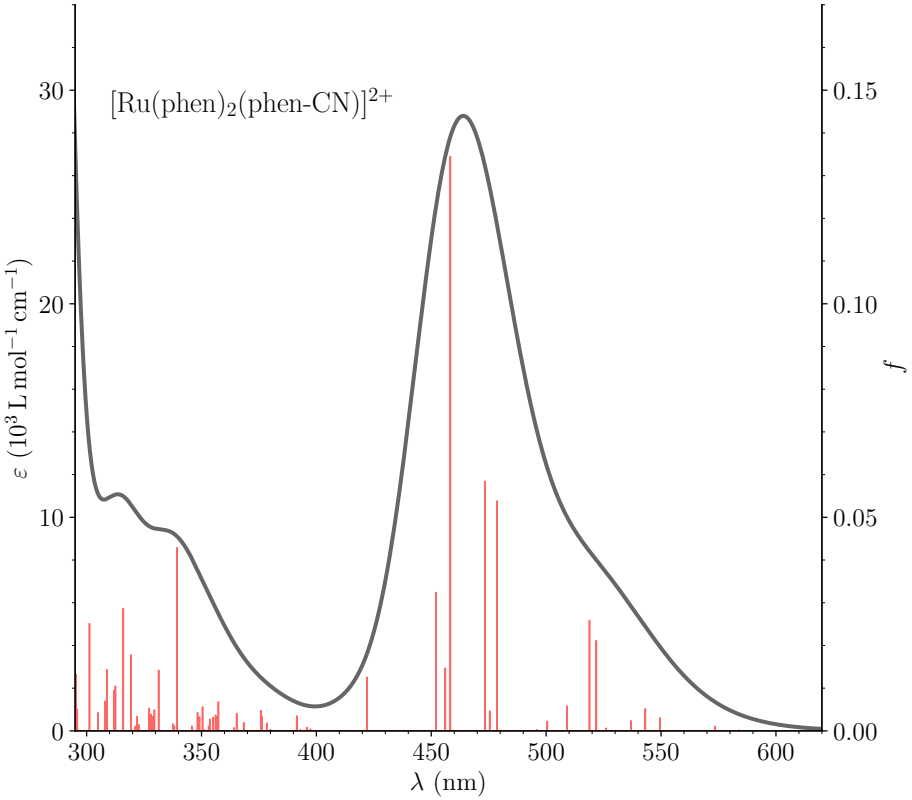
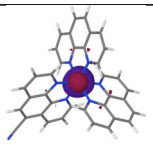
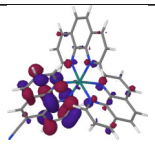
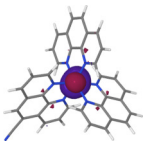
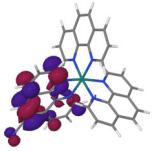
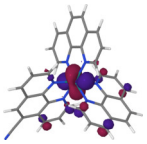
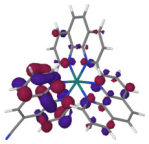
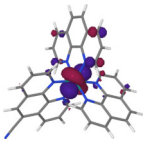
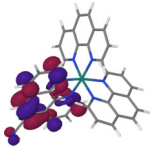
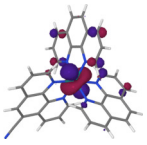
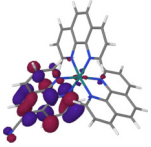
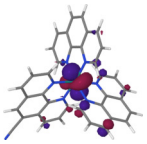
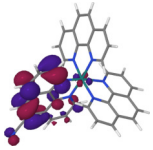
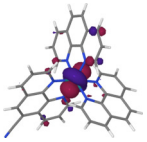
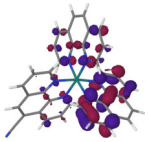
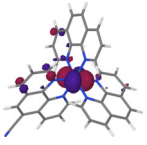
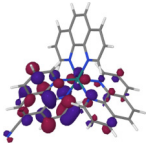
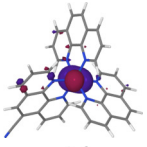
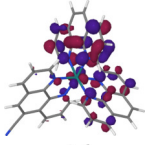
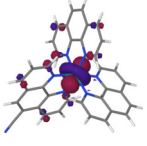
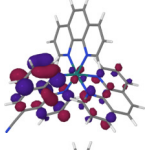
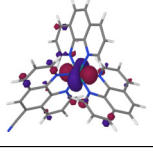
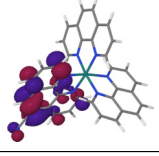


Figure S27: Absorption spectrum of $[Ru(phen)_2(phen\text{-}CN)]^{2+}$ obtained by convoluting the calculated oscillators strengths f with Gaussian having a full-with-at-half-maximum of 2000 cm^{-1} (SAOP/TZ2P results).

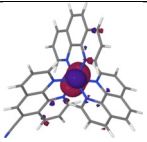
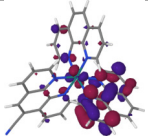
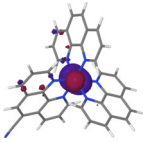
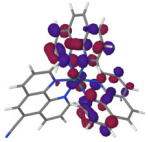
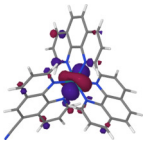
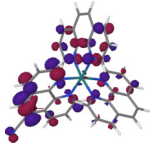
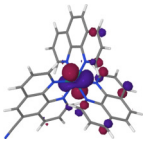
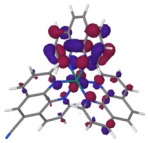
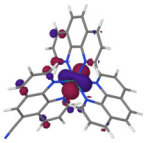
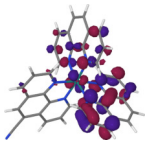
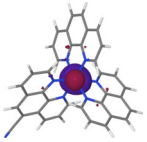
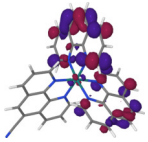
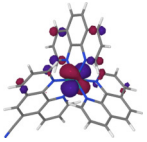
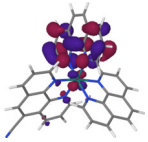
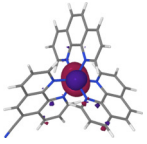
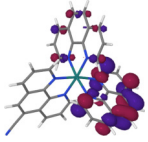
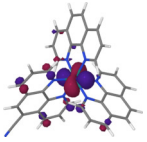
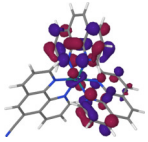
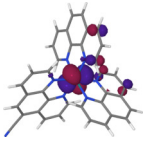
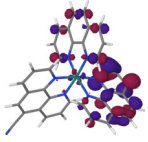
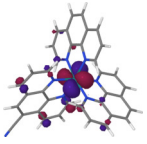
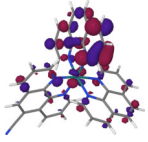
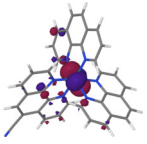
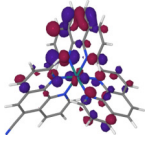
S10.3 Analysis of the electronic absorption spectrum

Table S4: Features of the $S_0 \rightarrow S_n$ electronic transition in $[Ru(phen)_2(phen\text{-}CN)]^{2+}$: transition wavelength λ, oscillator strength f, description in terms of natural transition orbitals (NTO) with the weights ω of NTO $\rightarrow$ NTO transitions (SAOP/TZ2P results)

Nr	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
1	584	0.000	99			
2	573	0.001	92			
3	550	0.003	63			
			31			
4	543	0.005	97			
5	537	0.002	55			
			30			
			14			
6	526	0.001	72			
			24			
7	522	0.021	55			

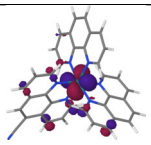
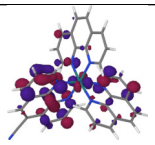
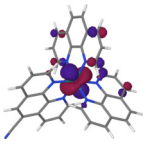
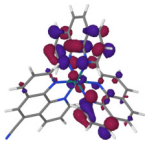
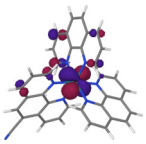
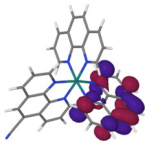
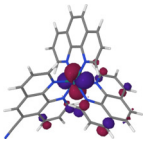
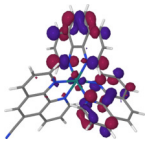
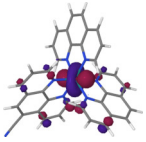
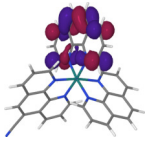
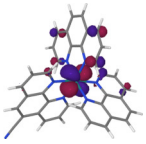
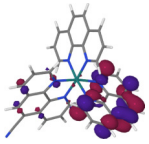
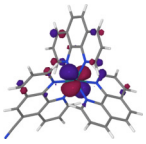
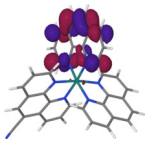
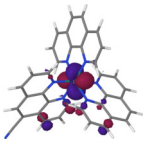
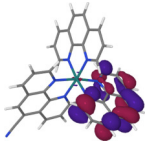
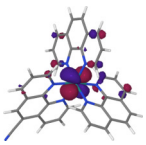
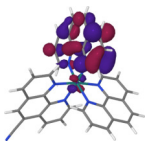
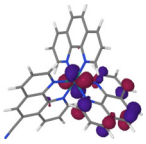
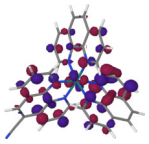
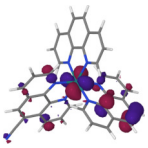
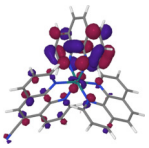
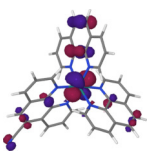
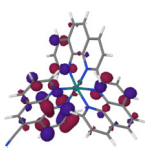
To be continued

Table S4 *continued*

Nr	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
			42			
8	519	0.026	64			
			35			
9	509	0.006	58			
			35			
10	500	0.002	79			
			19			
11	496	0.000	62			
			32			
12	479	0.054	49			
			27			
			20			

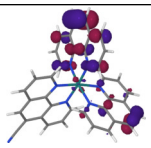
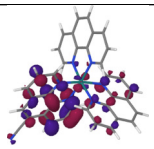
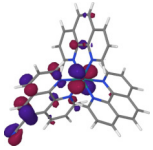
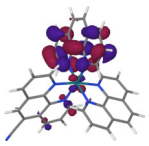
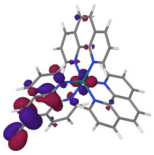
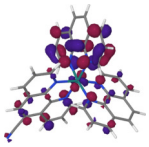
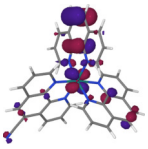
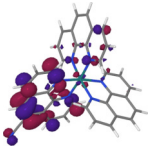
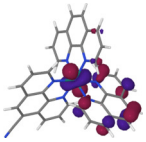
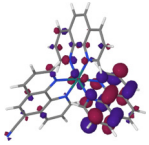
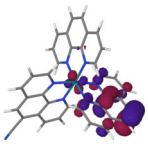
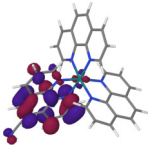
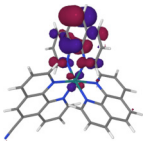
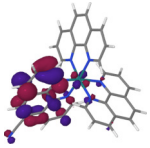
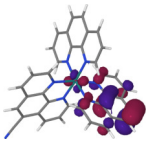
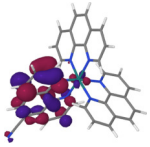
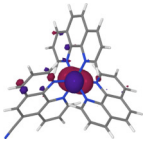
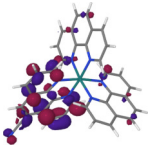
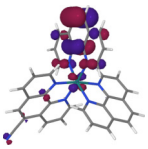
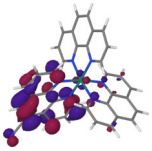
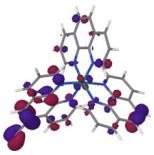
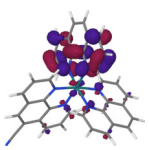
To be continued

Table S4 *continued*

Nr	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
13	475	0.005	49			
			43			
14	473	0.058	84			
			15			
15	458	0.135	85			
			12			
16	456	0.015	91			
17	452	0.032	77			
			18			
18	422	0.013	40			
			22			
			12			

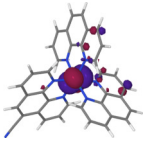
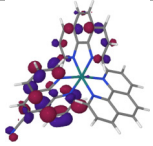
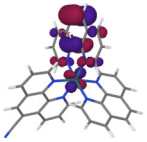
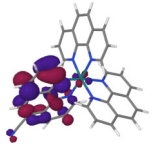
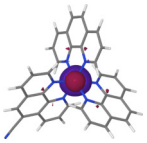
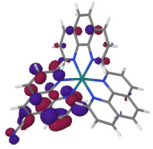
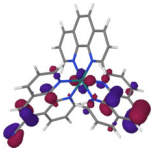
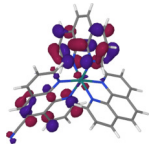
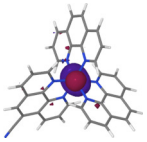
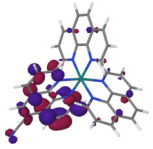
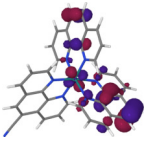
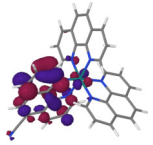
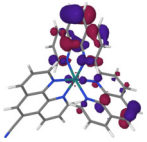
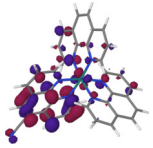
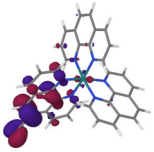
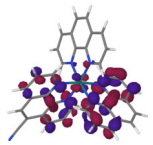
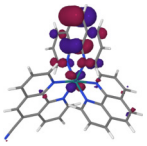
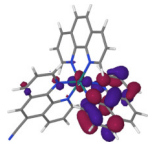
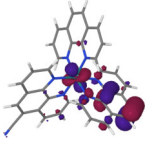
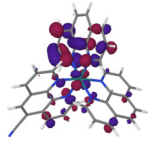
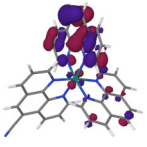
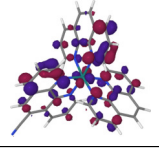
To be continued

Table S4 *continued*

Nr	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
19	397	0.000	57			
			19			
20	396	0.001	49			
			26			
			13			
21	393	0.000	73			
			22			
22	391	0.003	79			
			10			
23	380	0.000	54			
			20			

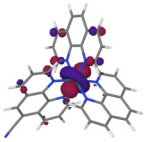
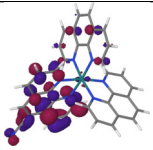
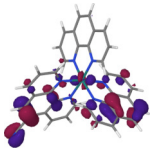
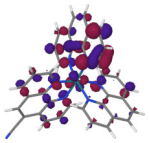
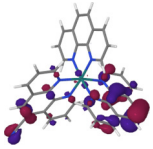
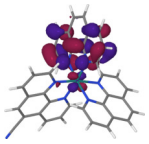
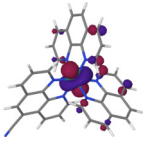
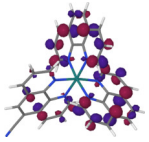
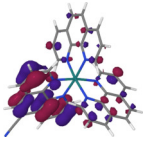
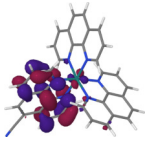
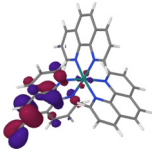
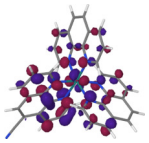
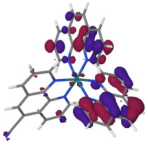
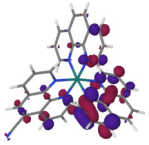
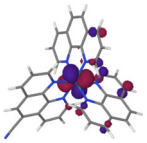
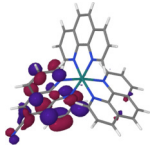
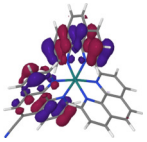
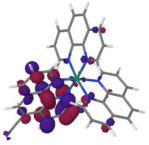
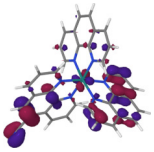
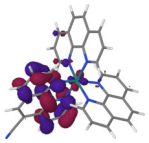
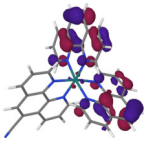
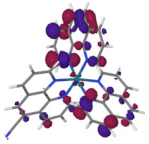
To be continued

Table S4 *continued*

Nr	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
			14			
24	379	0.002	43			
			28			
			20			
25	376	0.003	43			
			32			
			14			
26	376	0.005	71			
27	368	0.002	63			
			15			
28	365	0.004	23			

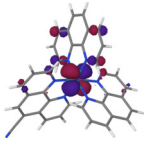
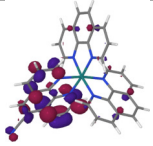
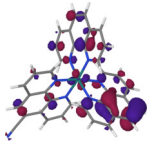
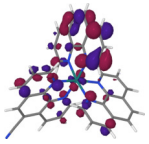
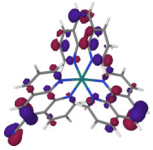
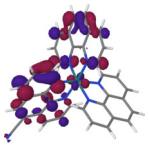
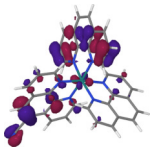
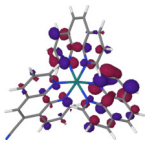
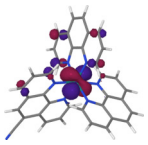
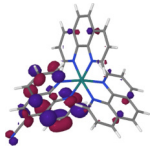
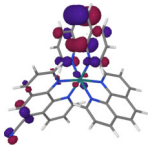
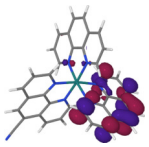
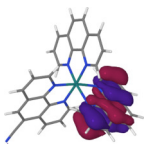
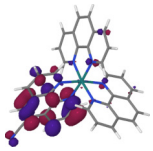
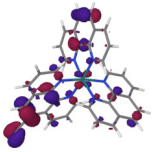
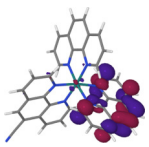
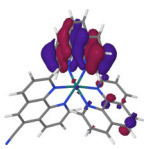
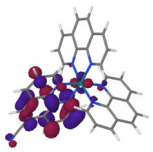
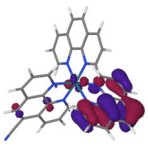
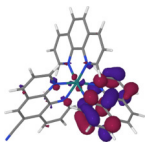
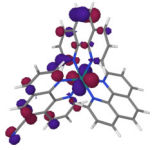
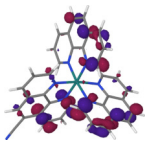
To be continued

Table S4 *continued*

Nr	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
			23			
			15			
29	364	0.001	47			
			25			
			15			
30	357	0.007	67			
			10			
31	357	0.001	51			
			17			
32	357	0.003	40			
			20			

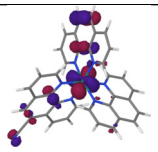
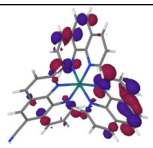
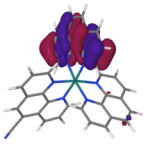
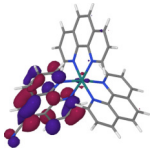
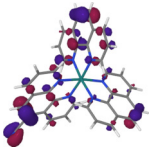
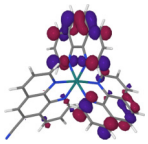
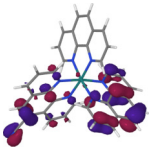
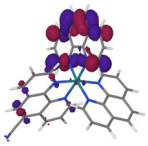
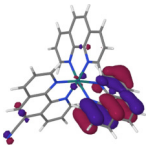
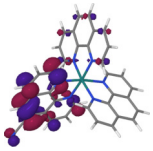
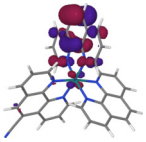
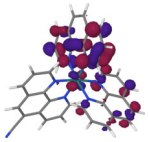
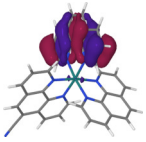
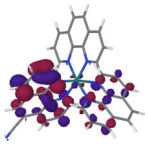
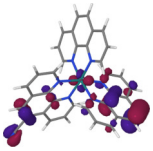
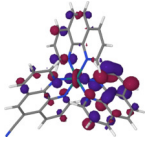
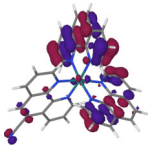
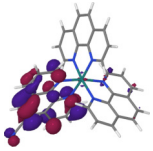
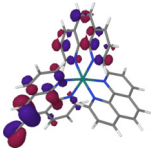
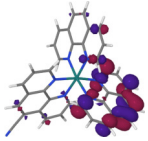
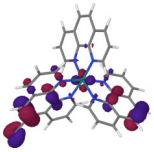
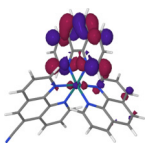
To be continued

Table S4 *continued*

Nr	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
			15			
33	356	0.004	37			
			15			
			11			
			11			
34	355	0.003	49			
			27			
35	354	0.003	45			
			23			
			20			
36	353	0.001	30			

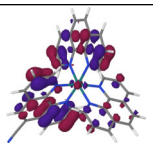
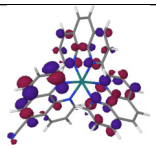
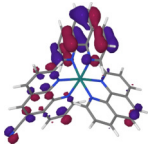
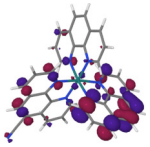
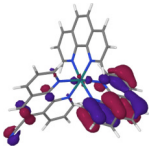
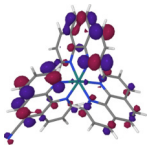
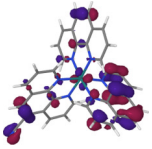
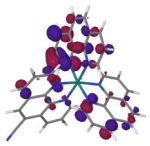
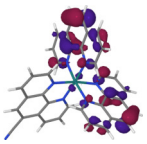
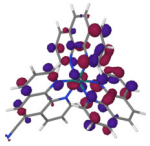
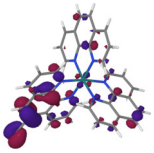
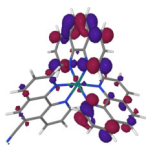
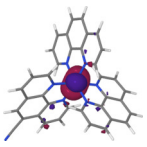
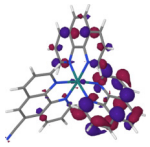
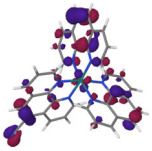
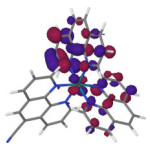
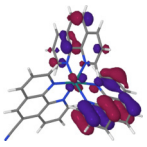
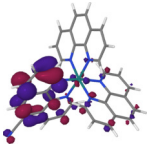
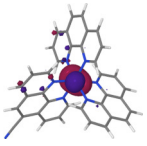
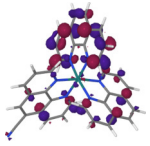
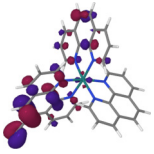
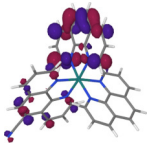
To be continued

Table S4 *continued*

Nr	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
			30			
			17			
			13			
37	351	0.000	42			
			34			
			13			
38	350	0.006	62			
			17			
39	349	0.003	51			
			21			
40	348	0.004	45			

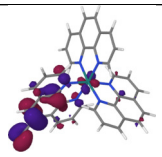
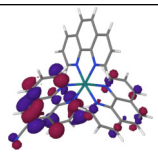
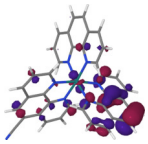
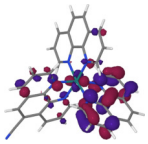
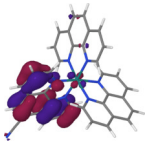
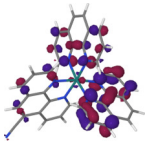
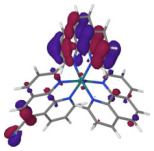
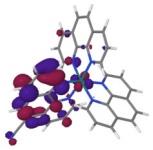
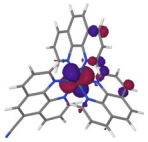
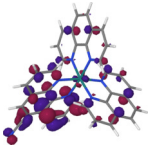
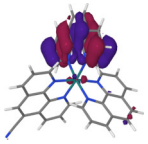
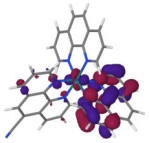
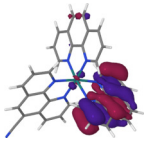
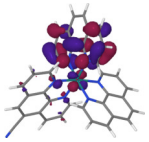
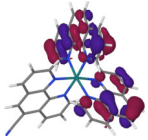
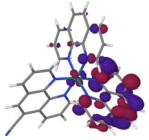
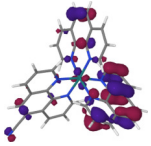
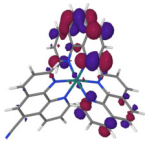
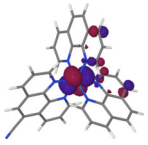
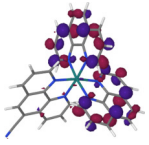
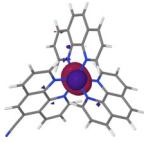
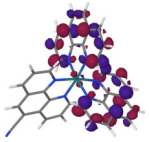
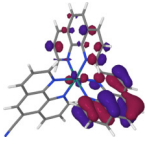
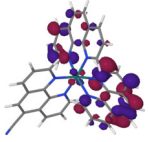
To be continued

Table S4 *continued*

Nr	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
			21			
			10			
41	346	0.001	38			
			25			
			16			
42	339	0.043	30			
			19			
			17			
			13			
43	338	0.001	69			
			14			

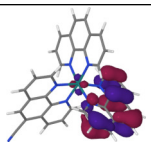
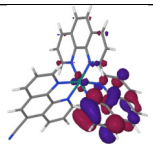
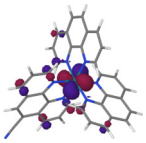
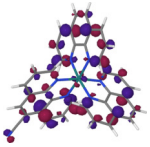
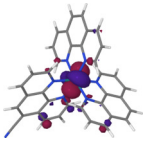
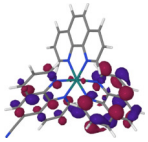
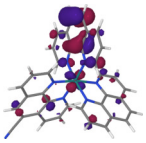
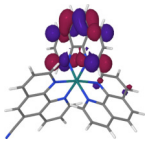
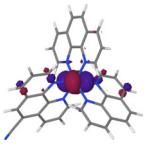
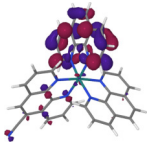
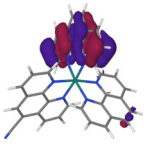
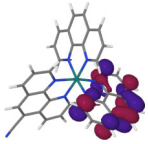
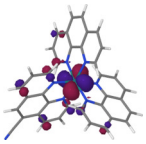
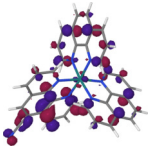
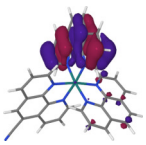
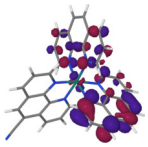
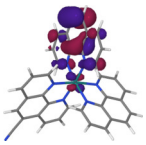
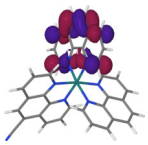
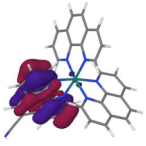
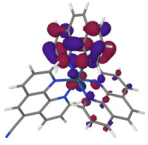
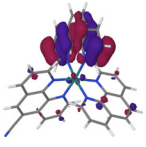
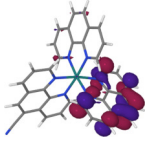
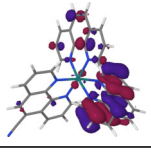
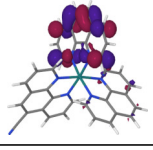
To be continued

Table S4 *continued*

Nr	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
44	338	0.002	54			
			18			
45	334	0.000	42			
			17			
			16			
46	331	0.014	92			
47	330	0.005	92			
48	329	0.003	33			
			26			
			18			
49	328	0.004	46			
			14			

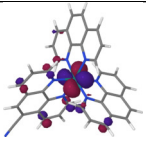
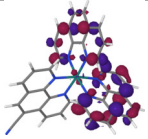
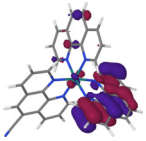
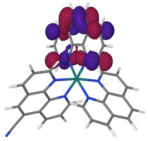
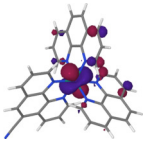
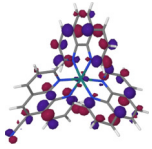
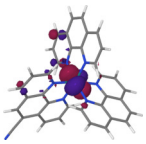
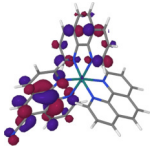
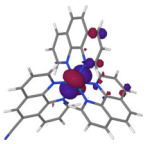
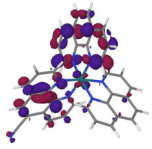
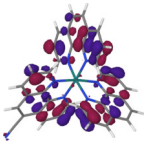
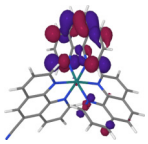
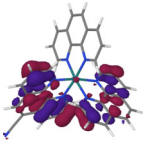
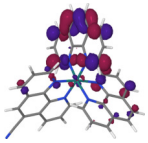
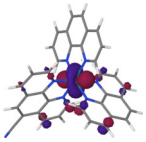
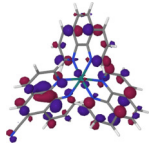
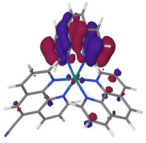
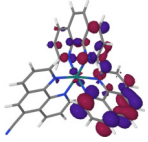
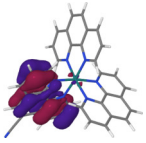
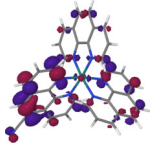
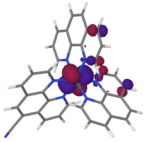
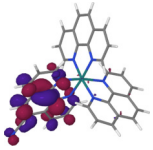
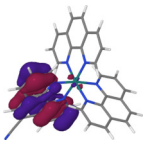
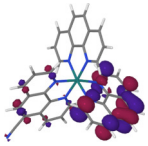
To be continued

Table S4 *continued*

Nr	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
			13			
			12			
50	327	0.005	25			
			22			
			20			
			18			
51	323	0.001	42			
			21			
			20			
52	322	0.003	80			
53	321	0.001	45			
			40			

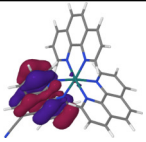
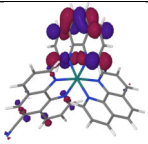
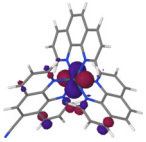
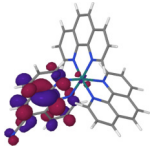
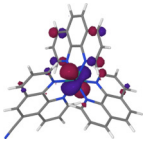
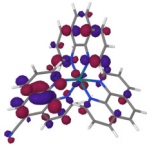
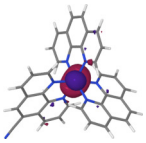
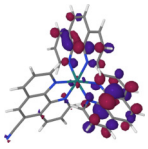
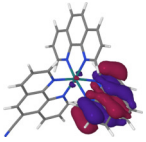
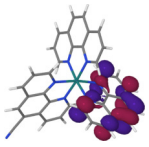
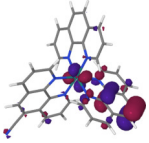
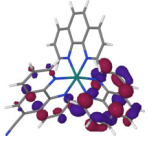
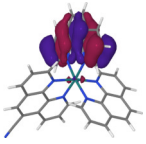
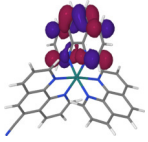
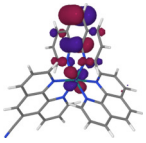
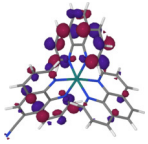
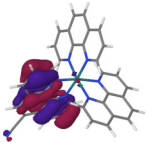
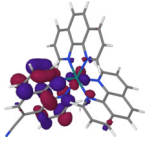
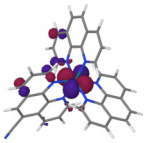
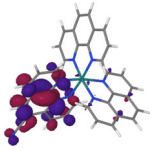
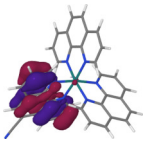
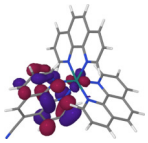
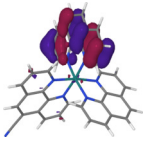
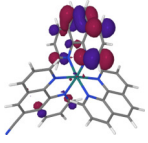
To be continued

Table S4 *continued*

Nr	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
54	319	0.018	56			
			18			
			10			
55	316	0.029	45			
			26			
			16			
56	313	0.010	43			
			29			
			14			
57	312	0.009	76			
58	309	0.014	85			
59	308	0.007	90			

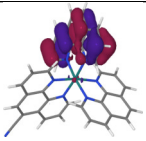
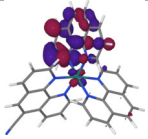
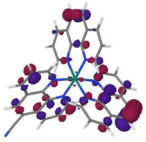
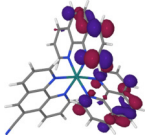
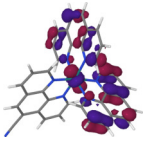
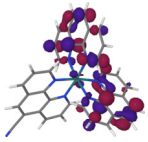
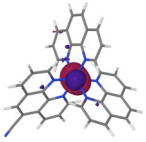
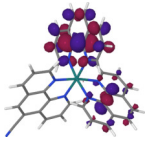
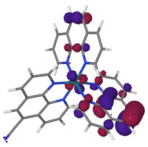
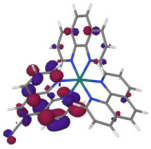
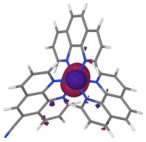
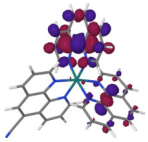
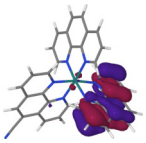
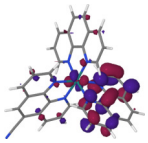
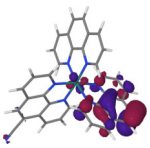
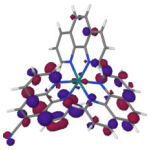
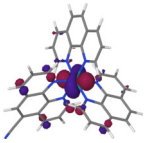
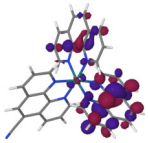
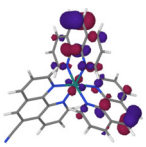
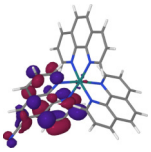
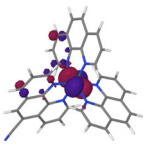
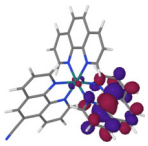
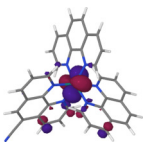
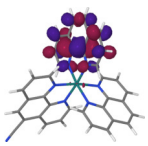
To be continued

Table S4 *continued*

Nr	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
60	305	0.004	50			
			42			
61	301	0.025	51			
			12			
62	296	0.005	59			
			25			
63	295	0.013	44			
			27			
			10			
64	290	0.004	28			
			22			
			16			

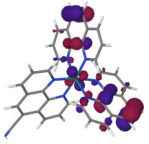
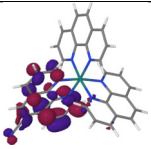
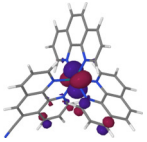
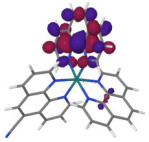
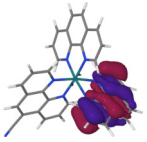
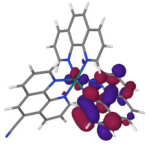
To be continued

Table S4 *continued*

Nr	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
65	288	0.133	34			
			15			
			12			
66	287	0.063	44			
			28			
67	286	0.015	46			
			15			
			13			
			10			
68	285	0.065	70			
69	284	0.037	59			
			21			

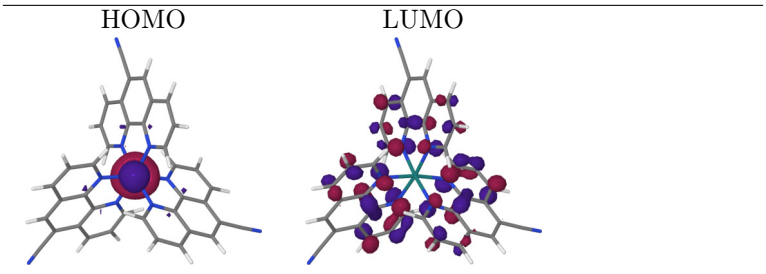
To be continued

Table S4 *continued*

Nr	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
70	282	0.063	40			
			20			
			18			

S11 Computational results: $[Ru(phen\text{-}CN)_3]^{2+}$

S11.1 HOMO-LUMO gap



S11.2 Calculated absorption spectrum

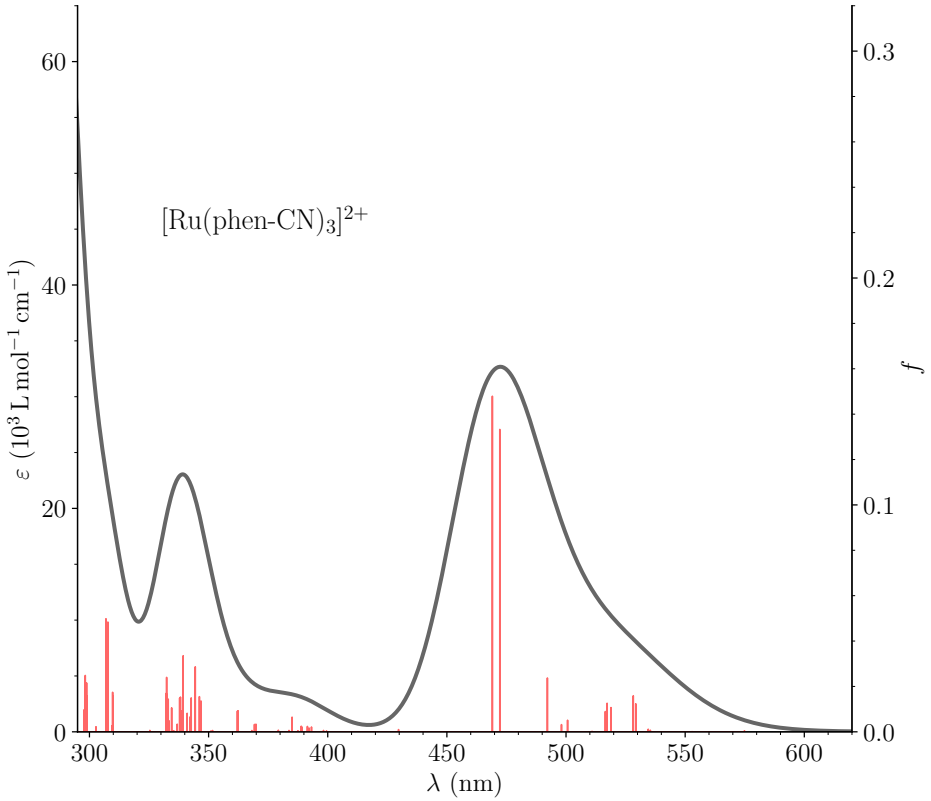
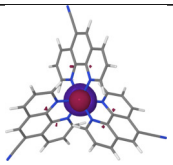
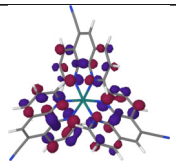
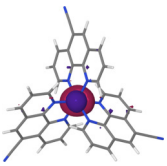
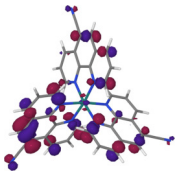
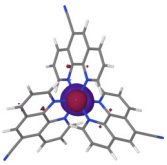
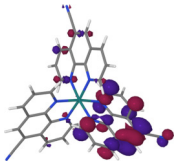
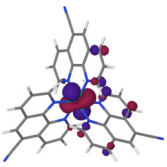
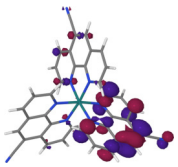
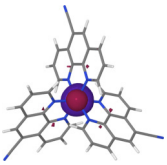
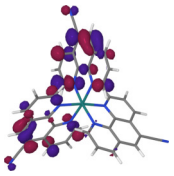
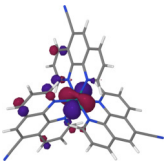
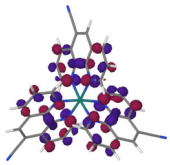
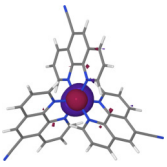
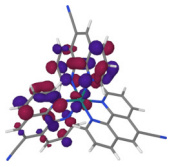
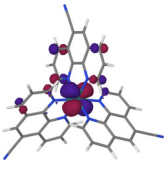
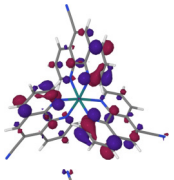
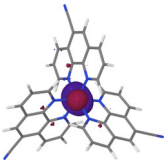
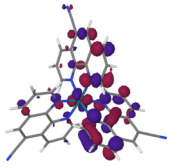


Figure S28: Absorption spectrum of $[Ru(phen\text{-}CN)_3]^{2+}$ obtained by convoluting the calculated oscillators strengths f with Gaussian having a full-with-at-half-maximum of 2000 cm^{-1} (SAOP/TZ2P results).

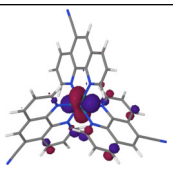
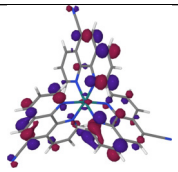
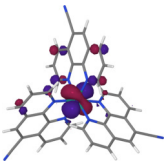
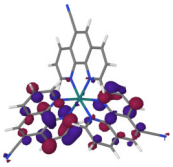
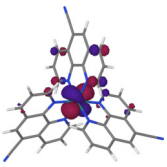
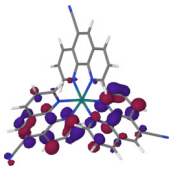
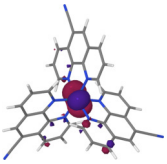
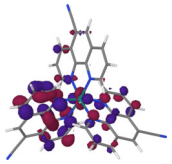
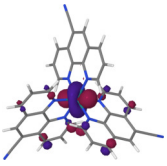
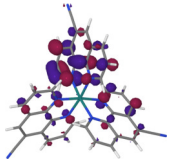
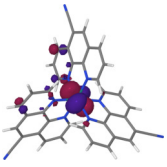
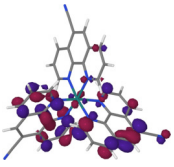
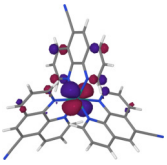
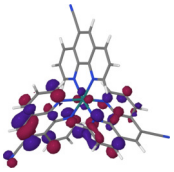
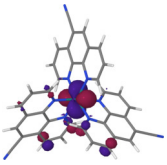
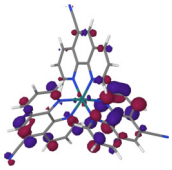
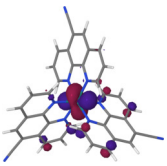
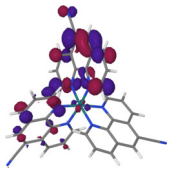
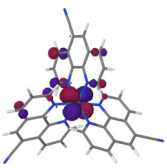
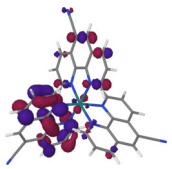
S11.3 Analysis of the electronic absorption spectrum

Table S5: Features of the $S_0 \rightarrow S_n$ electronic transition in $[Ru(phen\text{-}CN_2)_3]^{2+}$: transition wavelength λ, oscillator strength f, description in terms of natural transition orbitals (NTO) with the weights ω of NTO $\rightarrow$ NTO transitions (SAOP/TZ2P results).

n	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
1	575	0.000	99			
2	553	0.000	95			
3	547	0.000	86			
			14			
4	547	0.000	87			
			13			
5	535	0.001	79			
			17			
6	534	0.001	77			

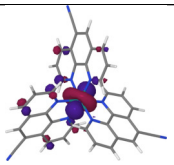
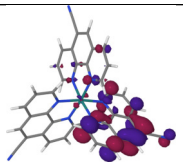
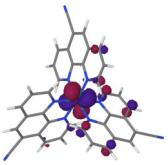
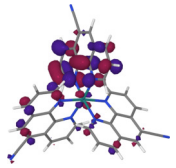
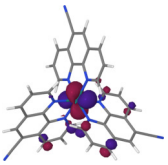
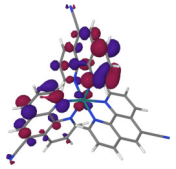
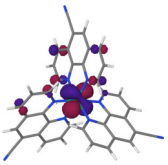
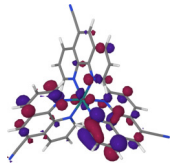
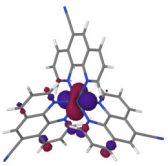
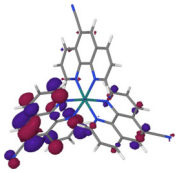
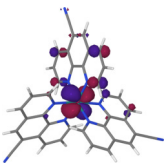
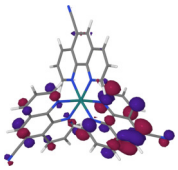
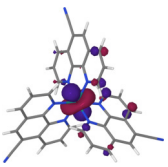
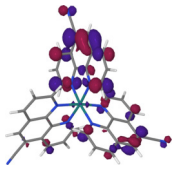
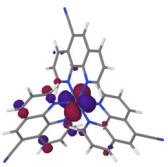
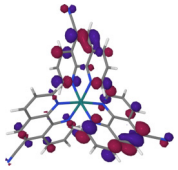
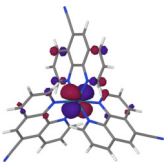
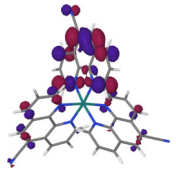
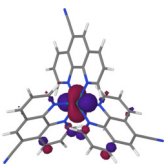
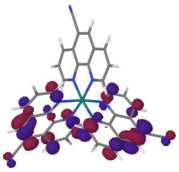
To be continued

Table S5: *continued*

n	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
			12			
			11			
7	529	0.012	62			
			32			
8	528	0.016	70			
			23			
9	519	0.011	73			
			22			
10	517	0.013	79			
			16			

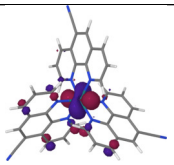
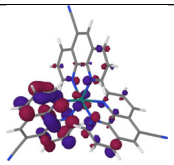
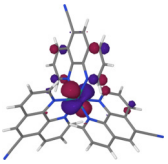
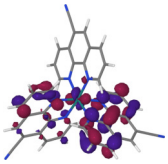
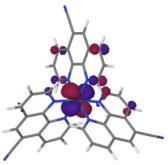
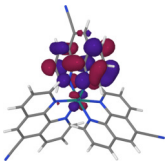
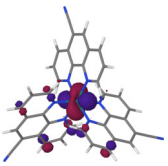
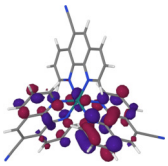
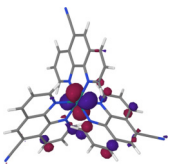
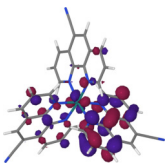
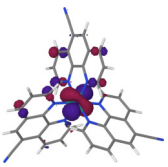
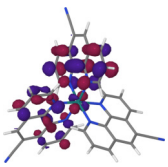
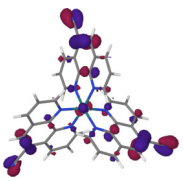
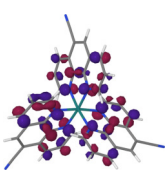
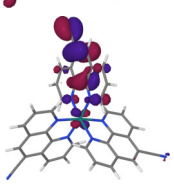
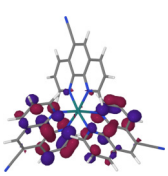
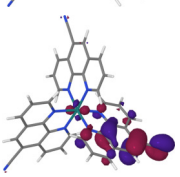
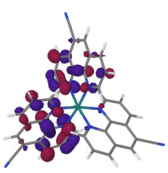
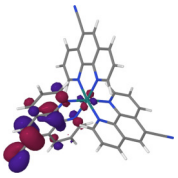
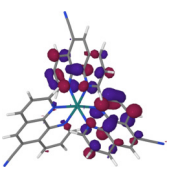
To be continued

Table S5: *continued*

n	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
11	516	0.009	73			
			23			
12	511	0.000	59			
			40			
13	501	0.005	61			
			35			
14	498	0.003	53			
			43			
15	492	0.024	56			
			39			

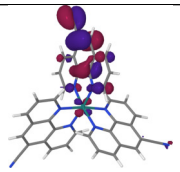
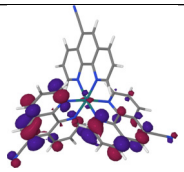
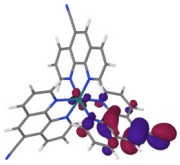
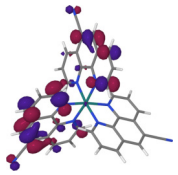
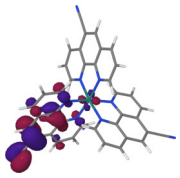
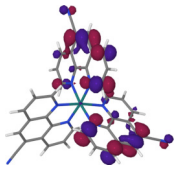
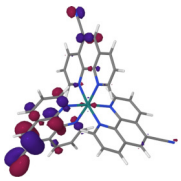
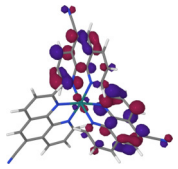
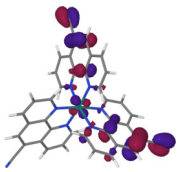
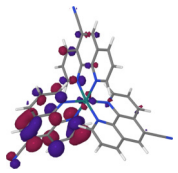
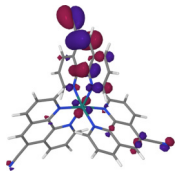
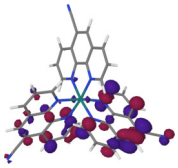
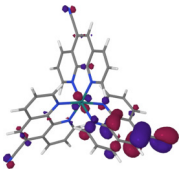
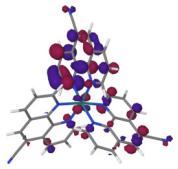
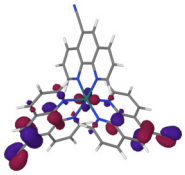
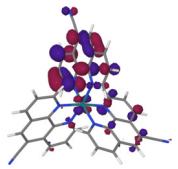
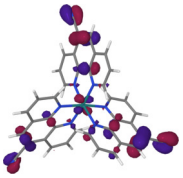
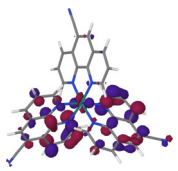
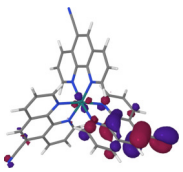
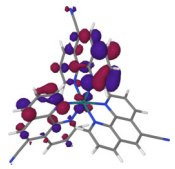
To be continued

Table S5: *continued*

n	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
16	472	0.133	53			
			42			
17	469	0.148	54			
			41			
18	430	0.001	39			
			38			
			10			
19	399	0.000	94			
20	398	0.001	91			
21	397	0.000	89			

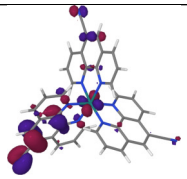
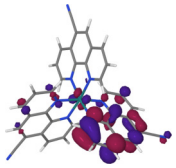
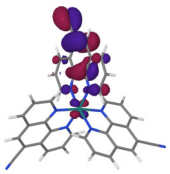
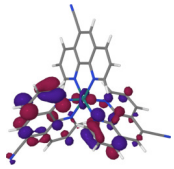
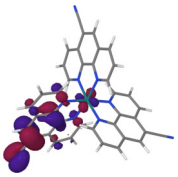
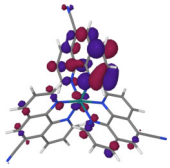
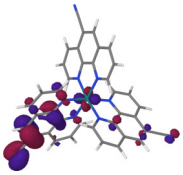
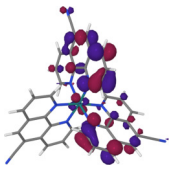
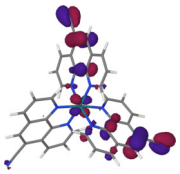
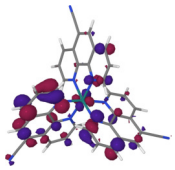
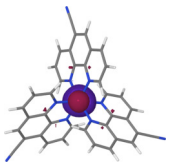
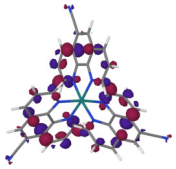
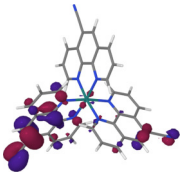
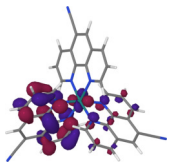
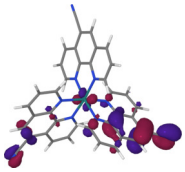
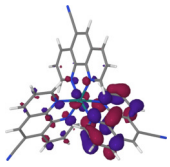
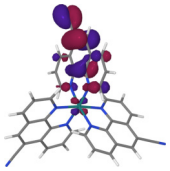
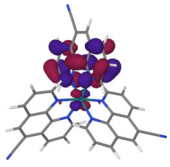
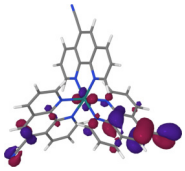
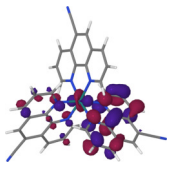
To be continued

Table S5: *continued*

n	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
22	393	0.002	93			
23	392	0.002	92			
24	391	0.002	90			
25	389	0.002	60			
			38			
26	389	0.002	64			
			30			
27	387	0.000	66			
			30			
28	385	0.006	83			

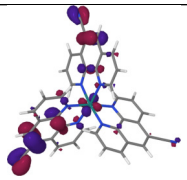
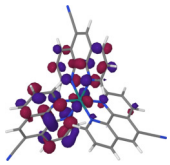
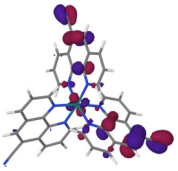
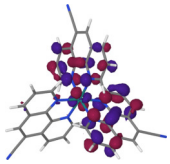
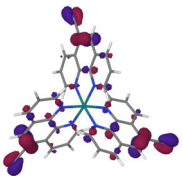
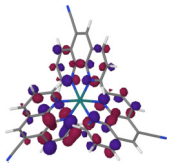
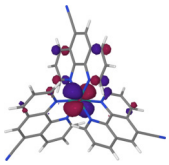
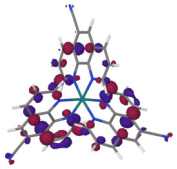
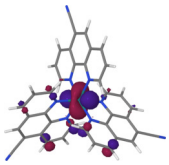
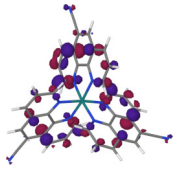
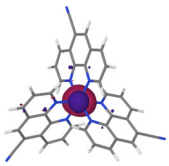
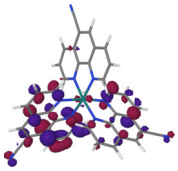
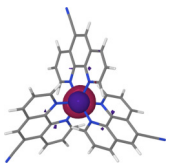
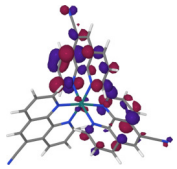
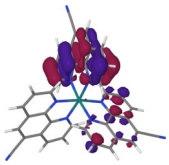
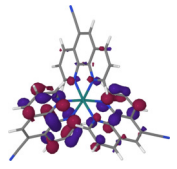
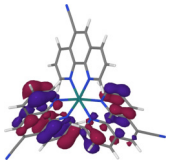
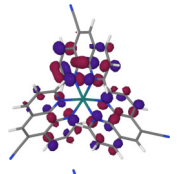
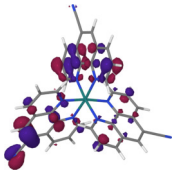
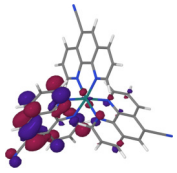
To be continued

Table S5: *continued*

n	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
			17			
29	385	0.006	87			
			11			
30	384	0.001	76			
			19			
31	379	0.001	92			
32	370	0.003	58			
			34			
33	369	0.003	59			
			29			

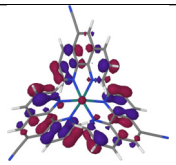
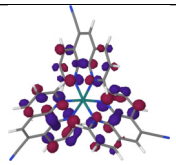
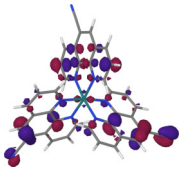
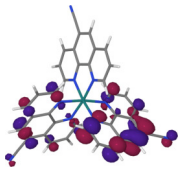
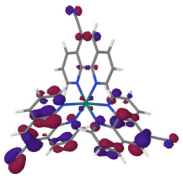
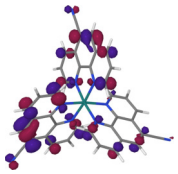
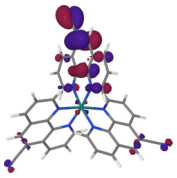
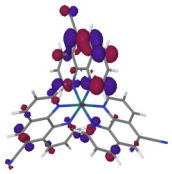
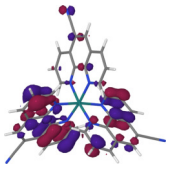
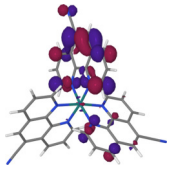
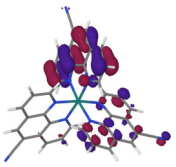
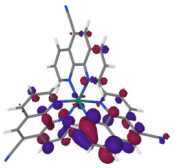
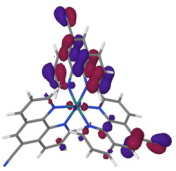
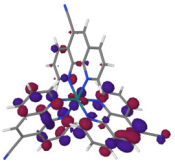
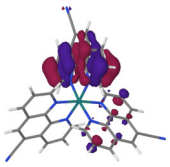
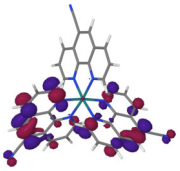
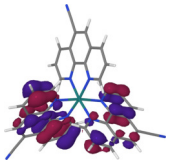
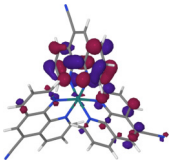
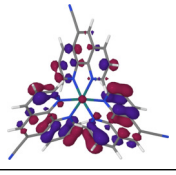
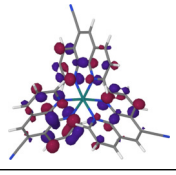
To be continued

Table S5: *continued*

n	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
34	368	0.001	43			
			40			
			10			
35	362	0.009	94			
36	362	0.009	94			
37	352	0.001	85			
38	351	0.000	82			
39	347	0.014	76			
40	346	0.016	62			
			17			

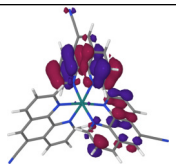
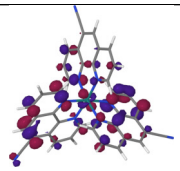
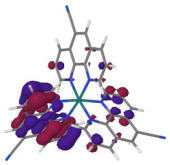
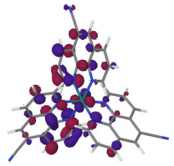
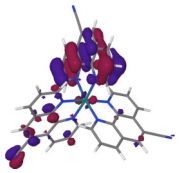
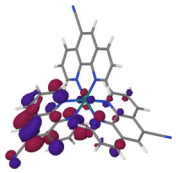
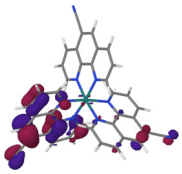
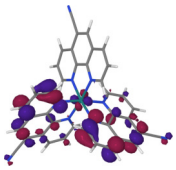
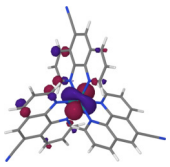
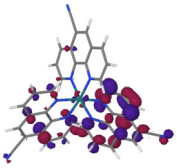
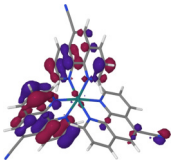
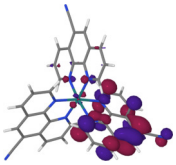
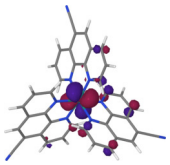
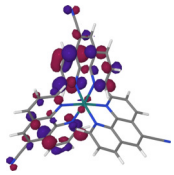
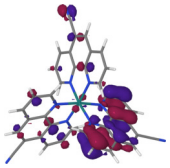
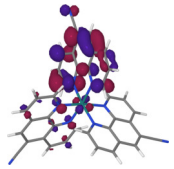
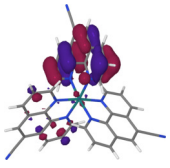
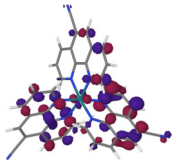
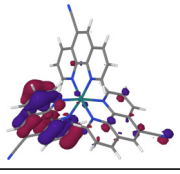
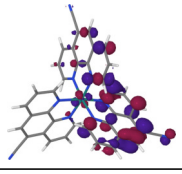
To be continued

Table S5: *continued*

n	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
41	344	0.029	29			
			27			
			17			
			13			
42	343	0.015	54			
			18			
			10			
43	342	0.007	51			
			24			
44	341	0.008	42			

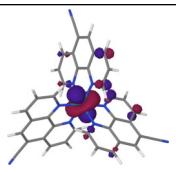
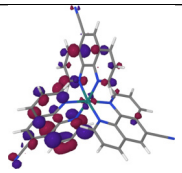
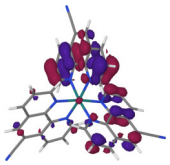
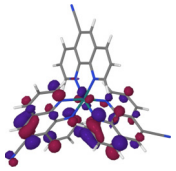
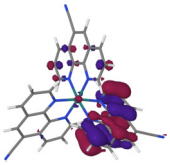
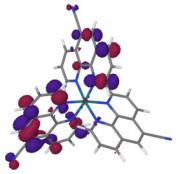
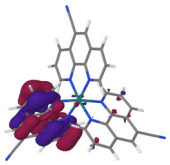
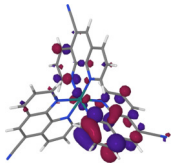
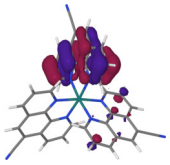
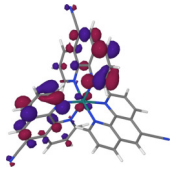
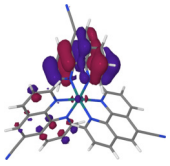
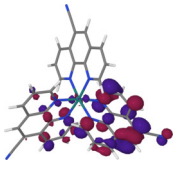
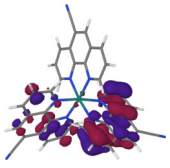
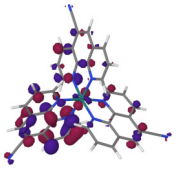
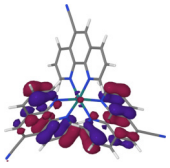
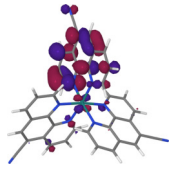
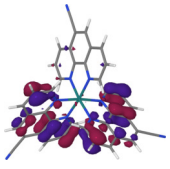
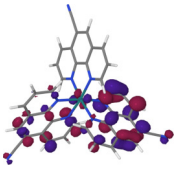
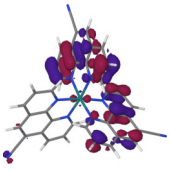
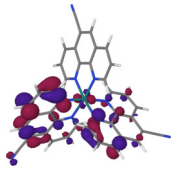
To be continued

Table S5: *continued*

n	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
			21			
			20			
45	339	0.034	67			
			11			
46	339	0.009	37			
			29			
			18			
47	338	0.015	71			
			11			
48	338	0.015	49			

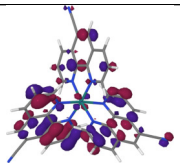
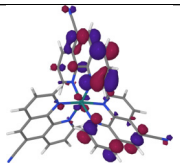
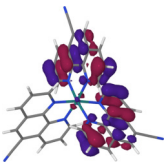
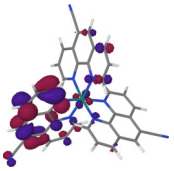
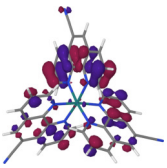
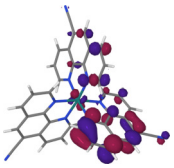
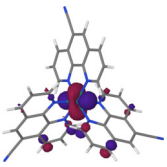
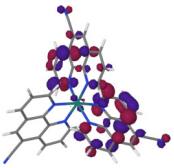
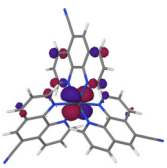
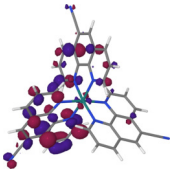
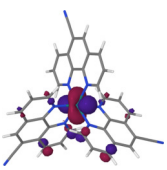
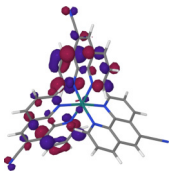
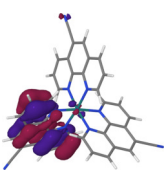
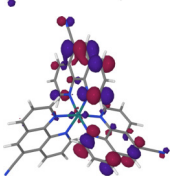
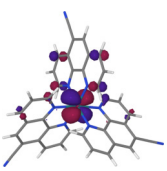
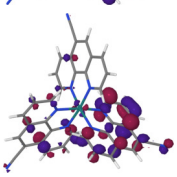
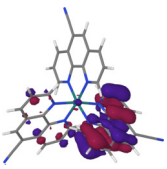
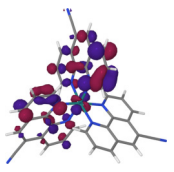
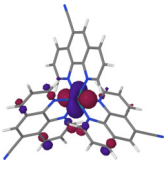
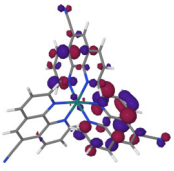
To be continued

Table S5: *continued*

n	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
			20			
			13			
49	337	0.003	55			
			27			
			11			
50	336	0.000	69			
			19			
51	335	0.000	73			
			13			
52	334	0.011	55			

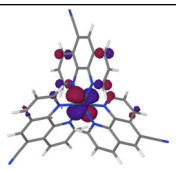
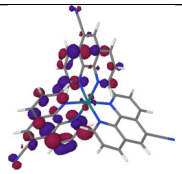
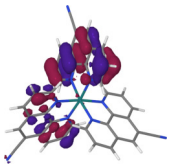
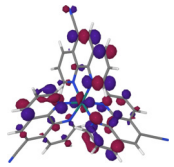
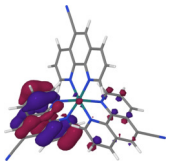
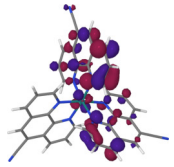
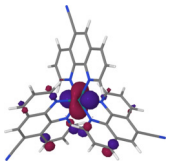
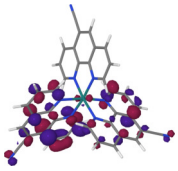
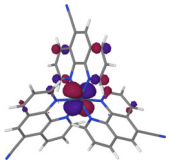
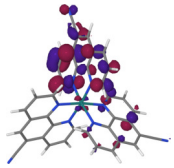
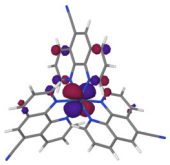
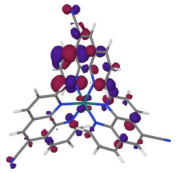
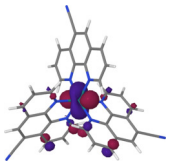
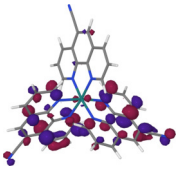
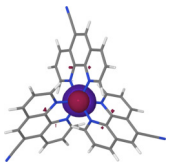
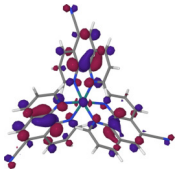
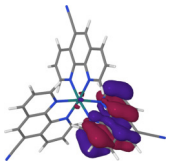
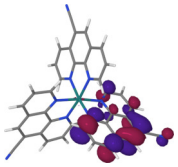
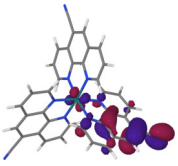
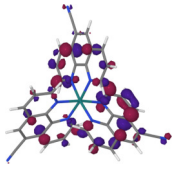
To be continued

Table S5: *continued*

n	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
			28			
53	333	0.005	51			
			25			
			11			
			10			
54	333	0.014	35			
			26			
			21			
55	332	0.024	34			
			23			

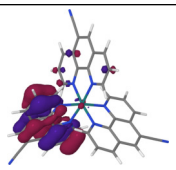
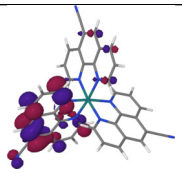
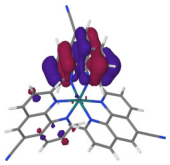
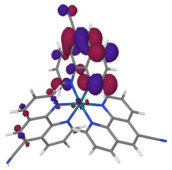
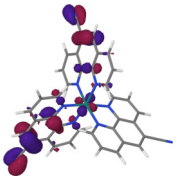
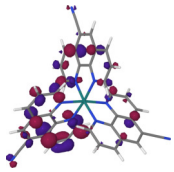
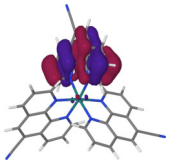
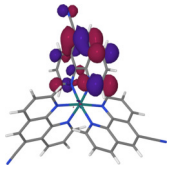
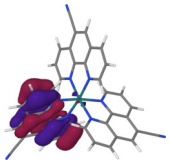
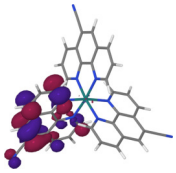
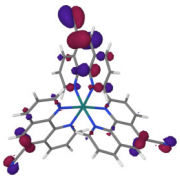
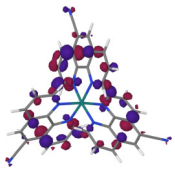
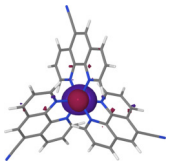
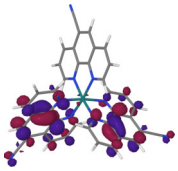
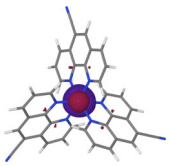
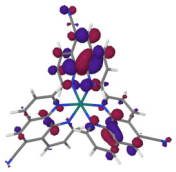
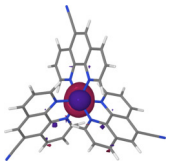
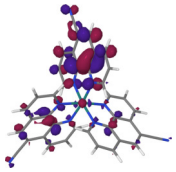
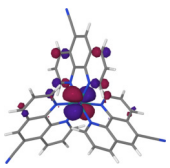
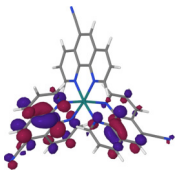
To be continued

Table S5: *continued*

n	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
			21			
			15			
56	332	0.017	53			
			18			
			15			
57	325	0.001	41			
			33			
			14			
58	310	0.016	61			
			10			

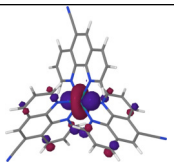
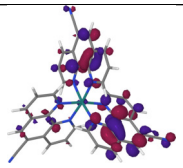
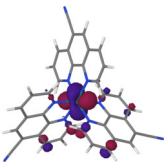
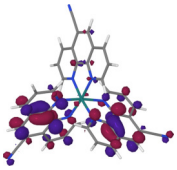
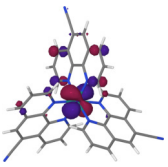
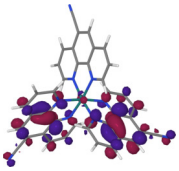
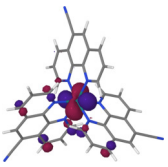
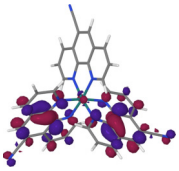
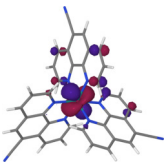
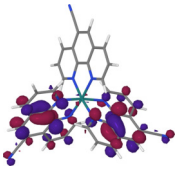
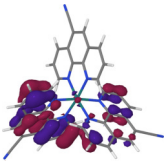
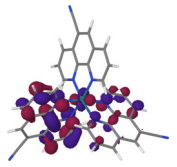
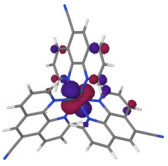
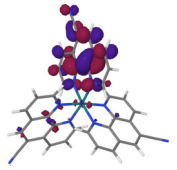
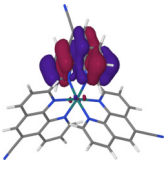
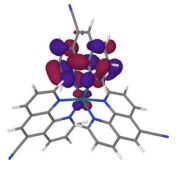
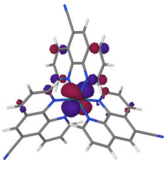
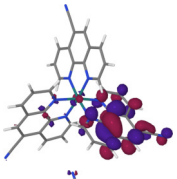
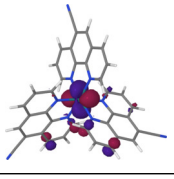
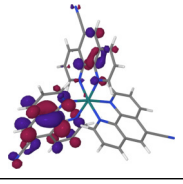
To be continued

Table S5: *continued*

n	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
59	310	0.017	49			
			20			
			11			
60	309	0.003	43			
			18			
			16			
61	308	0.048	82			
62	307	0.050	85			
63	303	0.002	46			
			27			

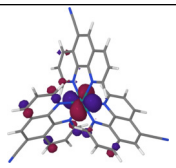
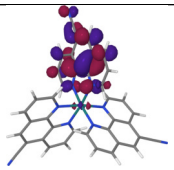
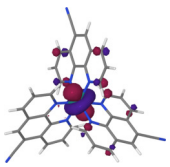
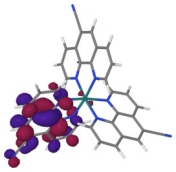
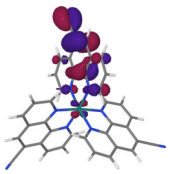
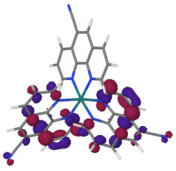
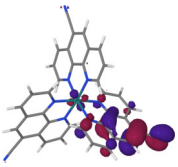
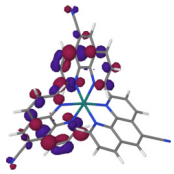
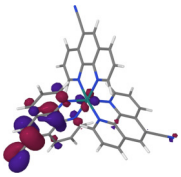
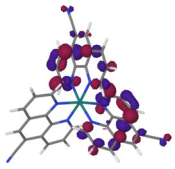
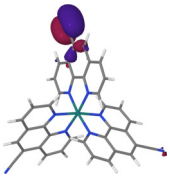
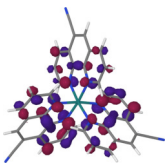
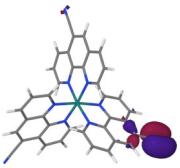
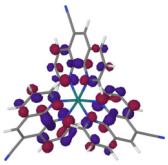
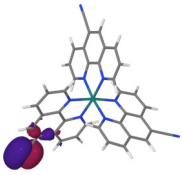
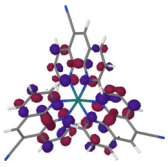
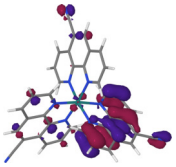
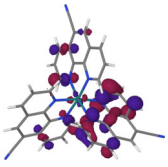
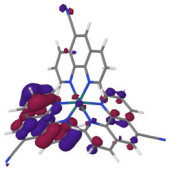
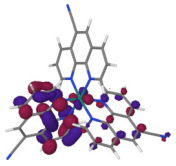
To be continued

Table S5: *continued*

n	λ (nm)	f	NTO			
			ω (%)	occ.	→	virt.
			24			
64	299	0.016	63			
			21			
65	299	0.022	55			
			21			
			11			
66	298	0.025	76			
			14			
67	298	0.010	65			
			28			

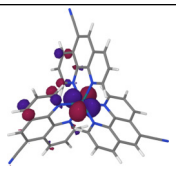
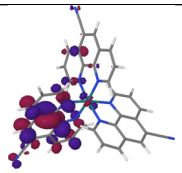
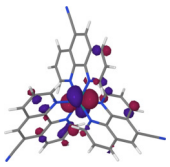
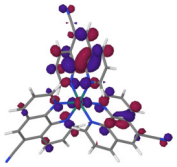
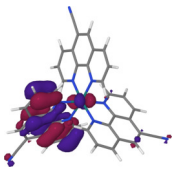
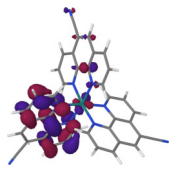
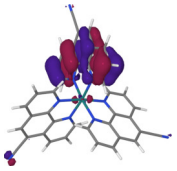
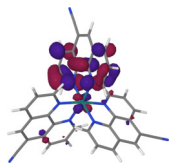
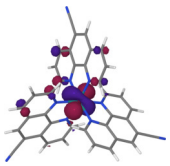
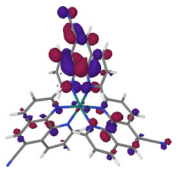
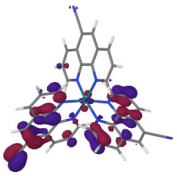
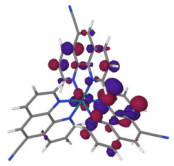
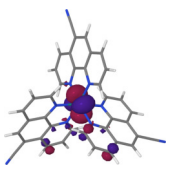
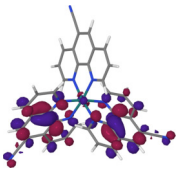
To be continued

Table S5: *continued*

n	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
68	298	0.010	67			
			28			
69	291	0.055	79			
70	291	0.085	77			
71	291	0.107	78			
72	288	0.001	100			
73	288	0.001	100			
74	287	0.001	99			
75	285	0.094	18			
			17			

To be continued

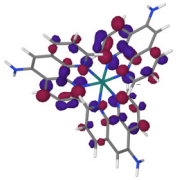
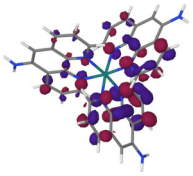
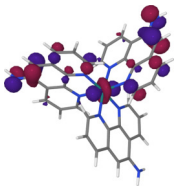
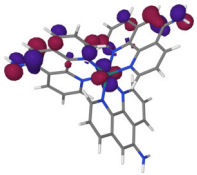
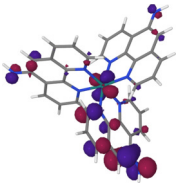
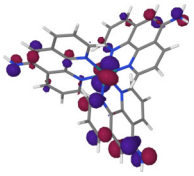
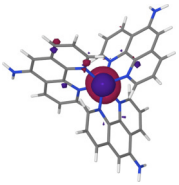
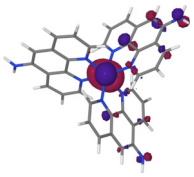
Table S5: *continued*

n	λ (nm)	f	NTO			
			ω (%)	occ.	$\rightarrow$	virt.
76	285	0.123	12			
			17			
			17			
77	285	0.088	26			
			12			
			12			
			11			

S12 Comparison of the computational results obtained for the *mer* and *fac* stereoisomers of $[Ru(phen\text{-}NH_2)_3]^{2+}$

The comparison of the computational results obtained for the frontiers orbitals (Section S12.1) and absorption spectra (Section S12.2) of the *mer* and *fac* stereoisomers of $[Ru(phen\text{-}NH_2)_3]^{2+}$ indicates that the mer/fac isomerism has a weak influence on the properties of the investigated the homoleptic complexes of substituted phen ligands.

S12.1 Frontier molecular orbitals

	fac-$[Ru(phen\text{-}NH_2)_3]^{2+}$	*mer*-$[Ru(phen\text{-}NH_2)_3]^{2+}$
LUMO		
	$\varepsilon_{LUMO} = -12.108$ eV	$\varepsilon_{LUMO} = -12.099$ eV
HOMO		
	$\varepsilon_{HOMO} = -14.147$ eV	$\varepsilon_{HOMO} = -14.117$ eV
HOMO-1		
	$\varepsilon_{HOMO-1} = -14.149$ eV	$\varepsilon_{HOMO-1} = -14.147$ eV
HOMO-2		
	$\varepsilon_{HOMO-2} = -14.181$ eV	$\varepsilon_{HOMO-2} = -14.172$ eV

The frontiers MOs of the two stereoisomers are very similar and their HOMO-LUMO gaps are very close: $\Delta\varepsilon_{fac} = 2.039$ eV and $\Delta\varepsilon_{mer} = 2.018$ eV (SR-SAOP/TZ2P results).

S12.2 Calculated absorption spectra

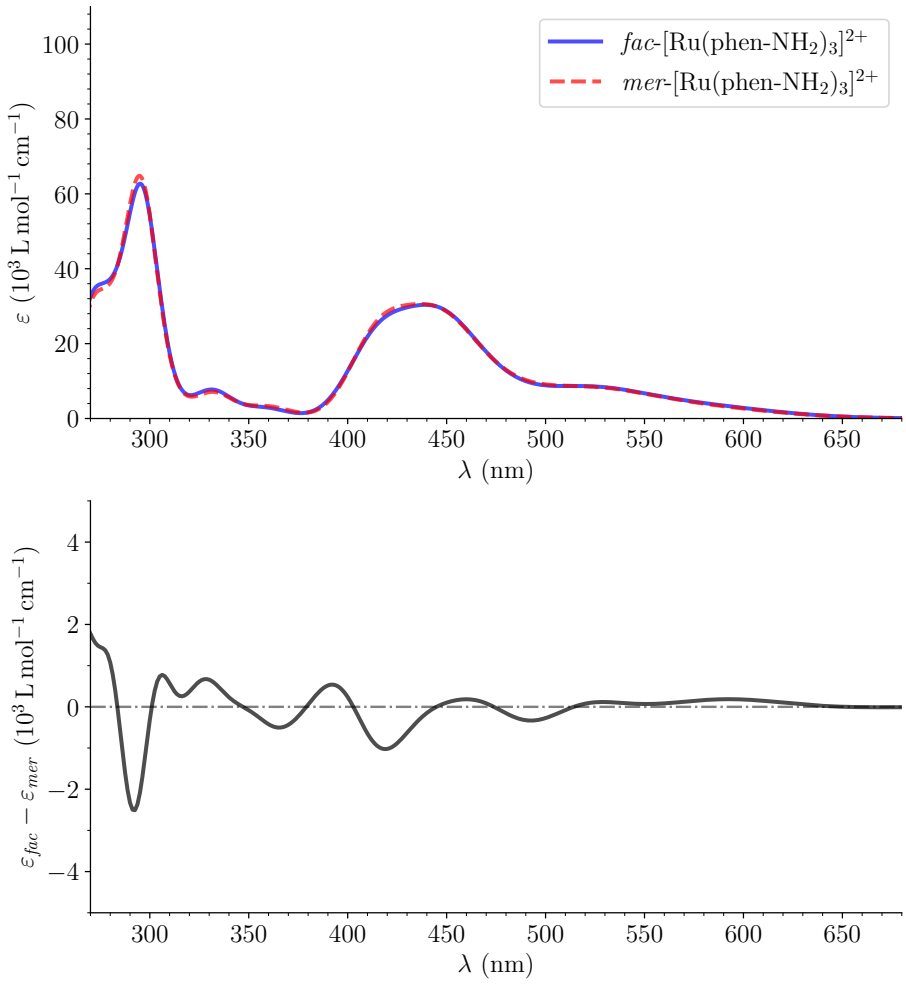


Figure S29: Comparison of the calculated absorption spectra of the *mer* and *fac* isomers of [Ru(phen-NH_2)$_3$]$^{2+}$: (Top) spectra obtained by convoluting the calculated oscillators strengths f with Gaussian having a full-with-at-half-maximum of 2000 cm^{-1}, (Bottom) the difference absorption spectrum (SAOP/TZ2P results).