Supplementary Information File:

Photophysical Properties of Pt (II) Complexes based on the Benzoquinoline (*bzq*) Ligand with OLED Implication: a Theoretical Study

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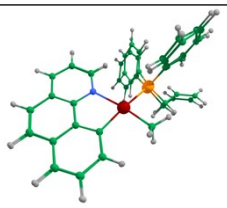
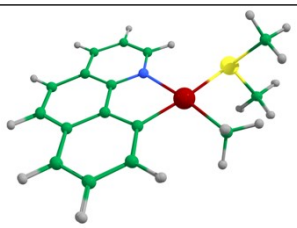
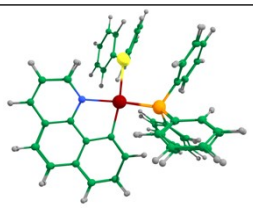
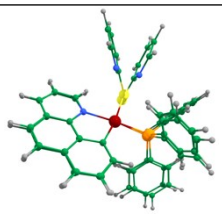
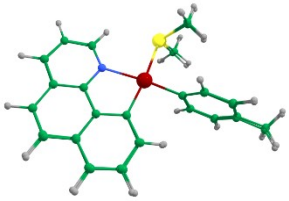
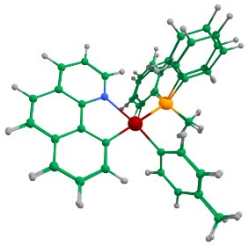
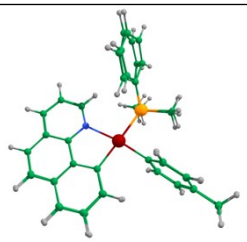
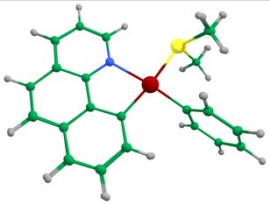
This supplementary file contains the following information:

1) Comparison of the S_0 and T_1 optimized geometries of our studied complexes.
2) Selected optimized geometry parameters of 3a-4a complexes in the S_0 and the T_1 states.
3) Electronic structures (MO contributions) of the studied complexes, determined at the SCF/cc-pVDZ/def2-TZVP (Pt) level of theory.
4) The vertical electronic transition energies of considered complexes (TD-DFT/B3LYP/cc-pVDZ/def2-TZVP(Pt) level of theory.
5) Optical properties and Exciton generation fractions χ_T (%) of selected systems
6) The XYZ coordinates of the optimized structure of our eight complexes.

Figure S1) Comparison the S_0 and T_1 optimized geometries of our studied complexes.

1a	1b	2a	2b
			
3a	**3b**	**3c**	**4a**
			

Complex	State	Bond length (Å)				Bond angle/degree			Dihedral angle/deg	
3a		Pt-N	Pt-C_1	Pt-C_2	Pt-S	N-Pt-C_1	N-Pt-C_2	C_1-Pt-S	C_1-N-Pt-S	N-C_1-Pt-C_2
	S_0	*2.201*	*2.027*	2.037	2.515	80.2	174.2	174.3	*180.0*	*179.7*
	T_1	*2.174*	*1.999*	*2.034*	*2.470*	*80.4*	*174.3*	*173.8*	*179.9*	*179.8*
	Exp.[39]	*2.142*	*2.052*	*2.029*	*2.358*	*80.9*	*173.7*	*174.8*	-	-
3b		Pt-N	Pt-C_1	Pt-C_2	Pt-P	N-Pt-C_1	N-Pt-C_2	C_1-Pt-P	C_1-N-Pt-P	N-C_1-Pt-C_2
	S_0	2.219	2.058	2.038	2.446	79.2	171.7	179.6	*179.9*	*179.9*
	T_1	2.188	2.037	2.038	2.393	79.5	171.8	178.7	*179.0*	*179.5*
	Exp.[40]	*2.136*	*2.054*	*2.008*	*2.301*	*80.2*	*170.4*	*176.7*	-	-
3c		Pt-N	Pt-C_1	Pt-C_2	Pt-P	N-Pt-C_1	N-Pt-C_2	C_1-Pt-P	C_1-N-Pt-P	N-C_1-Pt-C_2
	S_0	2.215	2.060	2.037	2.431	79.3	171.9	177.7	*178.3*	*177.7*
	T_1	2.184	2.037	2.038	2.383	79.6	172.1	176.8	*178.9*	*179.5*
	Exp.[40]	*2.145*	*2.041*	*2.013*	2.294	*80.4*	*170.9*	*176.4*	-	-
4a		Pt-N	Pt-C_1	Pt-C_2	Pt-S	N-Pt-C_1	N-Pt-C_2	C_1-Pt-S	C_1-N-Pt-S	N-C_1-Pt-C_2
	S_0	2.201	2.027	2.037	2.514	80.2	174.2	174.3	*180.0*	*179.8*
	T_1	2.125	1.195	2.017	2.438	80.4	174.5	173.7	*180.0*	*179.8*
	Exp.[41]	*2.128*	*2.030*	*2.009*	*2.358*	*81.5*	173.9	173.5	-	-

Table S1. *Selected optimized geometry parameters of **3a-4a** complexes in the S_0 and the T_1 states at the B3LYP level of theory. The experimental values obtained from the XRD structures have been adopted from the literature.[39-41] The C_2, P, S, and C_1 indicate bzq Carbon, Phosphorus, Sulfur, and Me carbon atoms connecting R_1 and R_2 ligands to central Pt.*

Table S2. Frontier molecular orbital contribution (%) in the ground state for complexes ***1a-4a***.

1a

Orbitals	E (eV)	Contribution (%)				Orbital interpretation (from high affect to minimum)
		Pt	bzq	Me	P-(Ph_2) (C_3H_5)	
HOMO-12	-7.522	12	45	-	43	π(bzq) + π($P(Ph)_2(C_3H_5)$) + d(Pt))
HOMO-7	-7.041	4	5	-	91	π($P(Ph)_2(C_3H_5)$)
HOMO-6	-6.588	38	42	1	19	π(bzq) + d(Pt) + π($P(Ph)_2(C_3H_5)$)
HOMO-5	-6.459	73	10	10	7	d(Pt) + π(bzq) + σ(Me)
HOMO-4	-6.370	14	41	2	43	[n(P) + π($Ph)_2(C_3H_5)$] + π(bzq) + d(Pt)
HOMO-3	-6.222	21	75	2	3	π(bzq) + d(Pt)
HOMO-2	-6.755	70	20	10	-	d(Pt) + π(bzq) + σ(Me)
HOMO-1	-6.533	85	9	6	-	dz^2(Pt)
HOMO	-5.374	26	72	-	2	π(bzq) + d(Pt)
LUMO	-1.598	4	96	-	-	π^*(bzq) most around N atom
LUMO+1	-1.112	4	56	-	40	π^*(bzq) + π^*($P(Ph)_2(C_3H_5)$)
LUMO+2	-0.981	2	29	-	68	π^*($P(Ph)_2(C_3H_5)$) + π^*(bzq)
LUMO+3	-0.861	1	5	1	93	π^*($P(Ph)_2(C_3H_5)$)
LUMO+4	-0.663	-	7	-	93	π^*($P(Ph)_2(C_3H_5)$)
LUMO+5	-0.368	2	-	-	98	π^*($P(Ph)_2(C_3H_5)$)
LUMO+6	-0.123	7	72	3	18	π^*(bzq) + π^*($P(Ph)_2(C_3H_5)$)
LUMO+7	-0.021	11	8	-	81	π^*($P(Ph)_2(C_3H_5)$) + π^*(bzq)

1b

Orbitals	E (eV)	Contribution (%)				Orbital interpretation (from high affect to minimum)
		Pt	bzq	Me	S-(Me_2)	
HOMO-9	-8.134	1	98	1	-	π(bzq)
HOMO-8	-7.615	19	79	1	1	π(bzq) + d(Pt)
HOMO-7	-7.138	16	38	30	16	π(bzq) + σ(Me) + d(Pt) + σ(S-Me_2)
HOMO-6	-6.786	16	30	13	41	π(bzq) + d(Pt) + σ(S-Me_2) + σ(Me)
HOMO-5	-6.606	40	59	-	1	π(bzq) + d(Pt)
HOMO-4	-6.298	76	6	8	10	d(Pt) + σ(S-Me_2)
HOMO-3	-6.277	16	83	1	-	π(bzq) + d(Pt)
HOMO-2	-5.741	74	19	7	-	d(Pt) + π(bzq)
HOMO-1	-5.527	91	5	4	-	dz^2(Pt)
HOMO	-5.387	28	70	-	2	π(bzq) + d(Pt)
LUMO	-1.651	4	96	-	-	π^*(bzq)
LUMO+1	-1.127	5	91	-	4	π^*(bzq)
LUMO+2	-1.166	11	80	1	8	π^*(bzq) + d(Pt)
LUMO+3	0.345	14	36	-	50	σ^*(S-Me_2) + π^*(bzq) + d(Pt)
LUMO+4	0.826	38	29	12	21	d(Pt) + π^*(bzq) + σ^*(S-Me_2) + σ^*(Me)
LUMO+5	0.933	2	87	-	11	π^*(bzq) + σ^*(S-Me_2)

2a

Orbitals	E (eV)	Contribution (%)				Orbital interpretation (from high affect to minimum)
		Pt	bzq	S-(Ph)	P-(Ph_3)	
HOMO-13	-7.247	4	2	-	94	$\pi(P(Ph)_3)$
HOMO-10	-6.976	47	15	18	20	$d(Pt) + \pi(P(Ph)_3) + \pi(S\text{-}Ph) + \pi(bzq)$
HOMO-9	-6.931	38	13	25	24	$d(Pt) + \pi(S\text{-}Ph) + \pi(P(Ph)_3) + \pi(bzq)$
HOMO-8	-6.867	7	4	2	87	$\pi(P(Ph)_3)$
HOMO-7	-6.822	38	46	9	7	$\pi(bzq) + d(Pt)$
HOMO-6	-6.651	3	3	30	64	$[n(S) + \pi(Ph)] + \pi(P(Ph)_3)$
HOMO-5	-6.363	15	83	-	2	$\pi(bzq) + d(Pt)$
HOMO-4	-6.259	14	1	81	4	$\pi(Ph) + dz^2(Pt)$
HOMO-3	-6.176	73	3	19	5	$dz^2(Pt) + \pi(Ph)$
HOMO-2	-5.915	8	34	55	3	$[n(S) + \pi(Ph)] + \pi(bzq)$
HOMO-1	-5.662	21	62	17	1	$\pi(bzq) + d(Pt) + n(S)$
HOMO	-4.564	6	3	89	2	$[n(S) + \pi(Ph)]$
LUMO	-1.883	4	94	-	2	$\pi^*(bzq)$ most around N atom
LUMO+1	-1.298	5	92	-	3	$\pi^*(bzq)$
LUMO+2	-1.091	-	3	-	97	$\pi^*(P(Ph)_3)$
LUMO+3	-0.919	15	6	5	74	$\pi^*(P(Ph)_3) + d(Pt)$
LUMO+4	-0.801	2	5	1	92	$\pi^*(P(Ph)_3)$
LUMO+5	-0.606	4	12	1	83	$\pi^*(P(Ph)_3) + \pi^*(bzq)$
LUMO+6	-0.485	4	13	1	82	$\pi^*(P(Ph)_3) + \pi^*(bzq)$
LUMO+7	-0.294	5	58	2	35	$\pi^*(bzq) + \pi^*(P(Ph)_3)$
LUMO+8	-0.063	1	4	4	91	$\pi^*(P(Ph)_3)$
LUMO+9	0.087	12	20	18	50	$\pi^*(P(Ph)_3) + \pi^*(bzq) + \pi^*(S\text{-}Ph) + d(Pt)$
LUMO+10	0.396	8	28	47	17	$\pi^*(S\text{-}Ph) + \pi^*(bzq) + \pi^*(P(Ph)_3)$

2b

Orbitals	E (eV)	Contribution (%)				Orbital interpretation (from high affect to minimum)
		Pt	bzq	S-(Py)	P-(Ph_3)	
HOMO-10	-6.977	19	4	41	36	$\pi(S\text{-}py) + \pi(P(Ph)_3) + d(Pt)$
HOMO-9	-6.839	45	12	14	29	$d(Pt) + \pi(P(Ph)_3) + \pi(S\text{-}py) + \pi(bzq)$
HOMO-8	-6.799	37	10	6	57	$\pi(P(Ph)_3) + d(Pt)$
HOMO-7	-6.748	37	49	5	9	$\pi(bzq) + d(Pt)$
HOMO-6	-6.684	7	4	16	73	$\pi(P(Ph)_3) + \pi(S\text{-}py)$
HOMO-5	-6.552	17	3	64	16	$\pi(S\text{-}py) + d(Pt) + \pi(P(Ph)_3)$
HOMO-4	-6.280	18	76	2	4	$\pi(bzq) + d(Pt)$
HOMO-3	-6.058	8	32	57	3	$\pi(S\text{-}py) + \pi(bzq)$
HOMO-2	-5.873	67	3	25	5	$d(Pt) + \pi(S\text{-}py)$
HOMO-1	-5.584	26	65	8	1	$\pi(bzq) + d(Pt)$
HOMO	-4.847	8	6	83	3	$[n(S) + \pi(py)]$
LUMO	-1.582	3	91	1	5	$\pi^*(bzq)$
LUMO+1	-1.221	4	91	1	4	$\pi^*(bzq)$
LUMO+2	-0.995	3	6	1	90	$\pi^*(P(Ph)_3)$
LUMO+3	-0.819	16	14	4	66	$\pi^*(P(Ph)_3) + d(Pt) + \pi^*(bzq)$
LUMO+4	-0.676	1	4	2	93	$\pi^*(P(Ph)_3)$
LUMO+5	-0.559	4	13	2	81	$\pi^*(P(Ph)_3) + \pi^*(bzq)$

LUMO+6	-0.386	4	19	3	74	$\pi^*(P(Ph)_3) + \pi^*(bzq)$
LUMO+7	-0.192	4	45	14	37	$\pi^*(bzq) + \pi^*(P(Ph)_3) + \pi^*(S\text{-}py)$
LUMO+8	-0.131	3	14	73	10	$\pi^*(S\text{-}py) + \pi^*(bzq) + \pi^*(P(Ph)_3)$
LUMO+9	-0.037	1	5	8	86	$\pi^*(P(Ph)_3)$
LUMO+10	0.196	8	16	39	37	$\pi^*(S\text{-}py) + \pi^*(P(Ph)_3) + \pi^*(bzq)$

3a

Orbitals	E (eV)	Contribution (%)				Orbital interpretation (from high affect to minimum)
		Pt	bzq	*p-Me*C_6H_4	S-(Me_2)	
HOMO-10	-7.732	22	76	1	1	$\pi(bzq) + d(Pt)$
HOMO-9	-7.312	24	34	24	18	$\pi(bzq) + d(Pt) + \pi\ (p\text{-}MeC_6H_4) + \sigma(S\text{-}Me_2)$
HOMO-8	-7.251	33	23	41	3	$\pi\ (p\text{-}MeC_6H_4) + d(Pt) + \pi(bzq)$
HOMO-7	-6.761	20	23	7	50	$\sigma(S\text{-}Me_2) + \pi(bzq) + d(Pt)$
HOMO-6	-6.728	40	53	2	6	$\pi(bzq) + d(Pt)$
HOMO-5	-6.398	30	65	5	-	$\pi(bzq) + d(Pt)$
HOMO-4	-6.188	9	1	87	3	$\pi\ (p\text{-}MeC_6H_4)$
HOMO-3	-6.044	55	36	8	1	$d(Pt) + \pi(bzq)$
HOMO-2	-5.643	85	6	8	1	d(Pt)
HOMO-1	-5.480	28	70	-	2	$\pi(bzq) + d(Pt)$
HOMO	-5.404	24	5	67	4	$\pi\ (p\text{-}MeC_6H_4) + d(Pt)$
LUMO	-1.758	4	94	2	0	$\pi^*(bzq)$
LUMO+1	-1.205	4	87	1	8	$\pi^*(bzq)$
LUMO+2	-0.232	8	72	5	15	$\pi^*(bzq) + \sigma^*(S\text{-}Me_2)$
LUMO+3	0.297	6	21	2	71	$\sigma^*(S\text{-}Me_2) + \pi^*(bzq)$
LUMO+4	0.412	4	7	82	7	$\pi^*(p\text{-}MeC_6H_4)$
LUMO+5	0.532	21	15	47	17	$\pi^*(p\text{-}MeC_6H_4) + d(Pt) + \sigma^*(S\text{-}Me_2) + \pi^*(bzq)$
LUMO+6	0.736	15	35	27	23	$\pi^*(bzq) + \pi^*(p\text{-}MeC_6H_4) + \sigma^*(S\text{-}Me_2) + d(Pt)$
LUMO+7	0.899	02	62	4	32	$\pi^*(bzq) + \sigma^*(S\text{-}Me_2)$

3b

Orbitals	E (eV)	Contribution (%)				Orbital interpretation (from high affect to minimum)
		Pt	bzq	*p-Me*C_6H_4	P-(Ph_2) (Me)	
HOMO-13	-7.528	9	28	4	59	$\pi(P(Ph)_2(Me)) + \pi(bzq)$
HOMO-12	-7.376	3	3	2	92	$\pi(P(Ph)_2(Me))$
HOMO-8	-7.086	20	30	35	15	$\pi\ (p\text{-}MeC_6H_4) + \pi(bzq) + d(Pt)+$
HOMO-7	-6.645	45	50	1	4	$\pi(bzq) + d(Pt)$
HOMO-6	-6.531	16	30	2	52	$\pi(P(Ph)_2(Me)) + \pi(bzq) + d(Pt)$
HOMO-5	-6.315	26	69	5	1	$\pi(bzq) + d(Pt)$
HOMO-4	-6.076	15	2	82	1	$\pi\ (p\text{-}MeC_6H_4) + d(Pt)$
HOMO-3	-5.994	53	32	14	1	$d(Pt) + \pi(bzq) + \pi\ (p\text{-}MeC_6H_4)$
HOMO-2	-5.532	82	7	9	2	d(Pt)
HOMO-1	-5.439	28	68	-	4	$\pi(bzq) + d(Pt)$
HOMO	-5.300	22	6	64	8	$\pi\ (p\text{-}MeC_6H_4) + d(Pt)$
LUMO	-1.583	4	93	2	1	$\pi^*(bzq)$

LUMO+1	-1.026	3	86	1	10	π^*(bzq)
LUMO+2	-0.994	3	4	1	92	π^*(P(Ph)$_2$(Me))
LUMO+3	-0.774	4	6	1	89	π^*(P(Ph)$_2$(Me))
LUMO+4	-0.637	4	7	-	89	π^*(P(Ph)$_2$(Me))
LUMO+5	-0.431	2	5	1	92	π^*(P(Ph)$_2$(Me))
LUMO+6	-0.084	8	73	5	14	π^*(bzq)
LUMO+10	0.895	12	23	53	12	π^*(*p*-MeC$_6$H$_4$)+π^*(bzq) + (Pt) + π^*(P(Ph)$_2$(Me))

3c

Orbitals	E (eV)	Contribution (%)				Orbital interpretation (from high affect to minimum)
		Pt	bzq	*p-Me*C$_6$H$_4$	P-(Ph) (Me$_2$)	
HOMO-11	-7.458	5	19	7	69	π(P(Ph)$_2$(Me)) + π(bzq)
HOMO-10	-7.371	4	4	2	90	π(P(Ph)$_2$(Me))
HOMO-9	-7.281	49	13	30	8	d(Pt) + π(*p*-MeC$_6$H$_4$) + π(bzq)
HOMO-8	-7.118	20	30	36	14	π(*p*-MeC$_6$H$_4$) + π(bzq) + d(Pt) + π(P(Ph)$_2$(Me))
HOMO-7	-6.663	44	49	2	5	π(bzq) + d(Pt)
HOMO-6	-6.610	18	35	2	44	π(P(Ph)$_2$(Me)) + π(bzq) + d(Pt)
HOMO-5	-6.329	25	70	5	-	π(bzq) + d(Pt)
HOMO-4	-6.100	13	2	84	1	π(*p*-MeC$_6$H$_4$) + d(Pt)
HOMO-3	-5.997	57	32	11	-	d(Pt) + π(bzq) + π(*p*-MeC$_6$H$_4$)
HOMO-2	-5.544	82	6	9	2	d(Pt)
HOMO-1	-5.449	28	69	-	3	π(bzq) + d(Pt)
HOMO	-5.319	22	6	64	8	π(*p*-MeC$_6$H$_4$) + d(Pt)
LUMO	-1.610	3	93	2	2	π^*(bzq)
LUMO+1	-1.042	3	86	2	9	π^*(bzq)
LUMO+2	-0.921	2	8	-	90	π^*(P(Ph)$_2$(Me))
LUMO+3	-0.616	5	5	1	89	π^*(P(Ph)$_2$(Me))
LUMO+4	-0.125	9	74	5	12	π^*(bzq) + π^*(P(Ph)$_2$(Me))
LUMO+5	0.551	6	25	30	39	π^*(P(Ph)$_2$(Me)) + π^*(*p*-MeC$_6$H$_4$) + π^*(bzq)
LUMO+6	0.587	9	24	48	19	π^*(*p*-MeC$_6$H$_4$) + π^*(P(Ph)$_2$(Me)) + π^*(bzq)
LUMO+7	0.712	13	27	17	43	π^*(P(Ph)$_2$(Me)) + π^*(bzq) + π^*(*p*-MeC$_6$H$_4$) +
LUMO+8	0.857	8	16	63	13	π^*(*p*-MeC$_6$H$_4$) + π^*(bzq) + π^*(P(Ph)$_2$(Me))

4a

Orbitals	E (eV)	Contribution (%)				Orbital interpretation (from high affect to minimum)
		Pt	bzq	Ph	S-(Me$_2$)	
HOMO-10	-7.746	20	79	-	1	π(bzq) + d(Pt)
HOMO-7	-6.760	17	22	6	55	σ(S-Me$_2$) + π(bzq) + d(Pt)
HOMO-6	-6.741	41	56	2	1	π(bzq) + d(Pt)
HOMO-5	-6.409	22	72	6	-	π(bzq) + d(Pt)
HOMO-4	-6.224	8	3	87	2	π(Ph)
HOMO-3	-6.064	65	28	7	-	d(Pt) + π(bzq)
HOMO-2	-5.613	76	4	19	1	d(Pt) + π(Ph)
HOMO-1	-5.576	44	6	45	5	π(Ph) + d(Pt)

HOMO	-5.514	31	66	-	2	π(bzq) + d(Pt)
LUMO	-1.657	3	95	2	-	π^*(bzq)
LUMO+1	-1.127	3	89	1	7	π^*(bzq)
LUMO+2	-0.183	8	72	5	15	π^*(bzq) + σ^*(S-Me_2)
LUMO+3	0.370	7	23	1	69	σ^*(S-Me_2) + π^*(bzq)
LUMO+4	0.430	28	26	26	20	d(Pt) + π^*(bzq) + π^*(Ph) + σ^*(S-Me_2)
LUMO+5	0.509	2	8	86	4	π^*(Ph)
LUMO+6	0.743	13	27	41	19	π^*(Ph) + π^*(bzq) + σ^*(S-Me_2) + d(Pt)
LUMO+7	0.948	2	57	4	37	π^*(bzq) + σ^*(S-Me_2)
HOMO-10	-7.746	20	79	-	1	π(bzq) + d(Pt)

Table S3. The vertical electronic transition energies of seven considered complexes:

1b

State	Major contribution (%)	E (eV)	*f*	λ_{cal} (nm)	Assignment
S_3	*H−2* → *L* (66.9%)	3.592	0.0817	345.2	^{1}MLCT/^{1}ILCT
S_7	*H* → *L+1* (81.1%)	3.916	0.0259	316.6	^{1}ILCT/^{1}MLCT
S_8	*H−4* → *L* (76.5%)	4.170	0.0419	297.4	^{1}MLCT/^{1}LLCT
S_9	*H−4* → *L+1* (44.4%)	4.335	0.0953	286	^{1}MLCT/^{1}LLCT
S_{12}	*H* → *L+2* (36.8%) *H−5* → *L* (35.5%) *H−2* → *L+2* (11.1%)	4.554	0.0500	272.3	^{1}ILCT/^{1}MLCT
S_{14}	*H−2* → *L+2* (96.8%)	4.783	0.0287	259.2	^{1}MLCT
S_{16}	*H−2* → *L+2* (50.4%) *H−5* → *L+1* (21.8%) *H* → *L+2* (14.1%)	4.867	0.0233	254.8	^{1}MLCT/^{1}ILCT
S_{17}	*H−5* → *L+1* (38.3%) *H−2* → *L+2* (21.5%)	4.980	0.1454	249	^{1}MLCT/^{1}ILCT
S_{18}	*H−1* → *L+4* (35.4%) *H−4* → *L+1* (11.2%)	5.097	0.5035	243.3	^{1}MLCT
S_{24}	*H* → *L+3* (70.9%)	5.296	0.0765	234.1	^{1}LLCT/^{1}MLCT
S_{25}	*H−1* → *L+3* (90.3%)	5.384	0.0678	230.3	^{1}MLCT
S_{26}	*H−8* → *L* (30.3%) *H−2* → *L+3* (26.9%) *H−3* → *L+4* (11.8%)	5.412	0.1103	229.1	^{1}ILCT/^{1}MLCT
S_{27}	*H−3* → *L+4* (65.5%) *H−2* → *L+3* (17.1%)	5.443	0.0383	227.8	^{1}LMCT/^{1}LLCT
S_{28}	*H−2* → *L+3* (44.2%) *H−8* → *L* (22.1%)	5.454	0.1450	227.3	^{1}MLCT/^{1}LLCT
S_{29}	*H−8* → *L+1* (29.2%) *H* → *L+5* (35.5%) *H−4* → *L+2* (19.2%)	5.676	0.0535	218.4	^{1}MLCT/^{1}LLCT
S_{31}	*H−5* → *L+2* (47.9%) *H* → *L+5* (31.6%)	5.814	0.1523	213.2	^{1}MLCT/^{1}LLCT
S_{37}	*H−4* → *L+2* (23.7%) *H−9* → *L+1* (35.5%) *H* → *L+5* (12.7%)	6.075	0.4203	204.1	^{1}MLCT/^{1}LLCT/^{1}ILCT
S_{44}	*H−4* → *L+3* (34.1%)	6.364	0.4919	194.8	^{1}MLCT/^{1}LLCT

2a

State	Major contribution (%)	E (eV)	*f*	λ_{cal} (nm)	Assignment
S_4	*H−1 → L (93.1%)*	3.261	0.075	380.2	^{1}MLCT/^{1}LLCT
S_{10}	*H−1 → L+1 (47.1%)* *H−4 → L (44.3%)*	3.831	0.032	323.6	^{1}MLCT/ ^{1}LLCT
S_{12}	*H−1 → L+3 (36.8%)* *H−1 → L+2 (22.7%)*	4.026	0.023	308	^{1}MLCT/ ^{1}LLCT

S_{13}	$H \rightarrow L+7$ (47.7%) $H \rightarrow L+9$ (12.0%)	4.035	0.103	307.3	^{1}LLCT
S_{14}	$H-1 \rightarrow L+1$ (22.3%)	4.088	0.100	303.3	^{1}MLCT/ ^{1}LLCT
S_{15}	$H \rightarrow L+8$ (59.0%) $H \rightarrow L+7$ (24.2%)	4.166	0.033	297.6	^{1}LLCT
S_{16}	$H-2 \rightarrow L+1$ (50.6%) $H-3 \rightarrow L+1$ (15.3%)	4.172	0.023	297.2	^{1}LLCT/^{1}MLCT
S_{18}	$H-1 \rightarrow L+2$ (36.9%) $H-1 \rightarrow L+3$ (22.8%)	4.208	0.029	294.6	^{1}LLCT/^{1}MLCT
S_{19}	$H-3 \rightarrow L+3$ (37.6%) $H-3 \rightarrow L+2$ (13.5%)	4.225	0.060	293.5	^{1}MLCT/ ^{1}LLCT
S_{21}	$H-3 \rightarrow L+1$ (25.0%) $H \rightarrow L+10$ (23.2%) $H-2 \rightarrow L+1$ (12.8%)	4.268	0.080	290.5	^{1}MLCT/^{1}LLCT
S_{24}	$H-9 \rightarrow L$ (60.2%)	4.417	0.073	280.7	^{1}MLCT/^{1}LLCT
S_{26}	$H-1 \rightarrow L+4$ (44.4%) $H-2 \rightarrow L+2$ (12.5%) $H-7 \rightarrow L$ (12.4%)	4.459	0.027	278.0	^{1}LLCT/^{1}MLCT
S_{27}	$H-1 \rightarrow L+4$ (29.2%) $H-2 \rightarrow L+2$ (25.8%) $H-2 \rightarrow L+3$ (20.0%)	4.489	0.135	276.2	^{1}LLCT/^{1}MLCT/^{1}LMCT
S_{29}	$H-1 \rightarrow L+5$ (25.7%) $H-2 \rightarrow L+3$ (11.2%) $H-7 \rightarrow L$ (11.1%)	4.591	0.088	270.1	^{1}MLCT/^{1}LLCT
S_{30}	$H-3 \rightarrow L+2$ (50.9%) $H-3 \rightarrow L+3$ (17.8%) $H-2 \rightarrow L+2$ (16.0%)	4.623	0.035	268.2	^{1}MLCT/^{1}LLCT
S_{33}	$H-1 \rightarrow L+5$ (19.9%) $H-8 \rightarrow L$ (12.9%)	4.683	0.054	264.8	^{1}MLCT/^{1}LLCT
S_{35}	$H-13 \rightarrow L$ (29.9%) $H-1 \rightarrow L+5$ (14.7%)	4.720	0.039	262.7	^{1}LLCT/^{1}MLCT
S_{36}	$H-10 \rightarrow L$ (31.8%) $H-1 \rightarrow L+5$ (15.3%) $H-4 \rightarrow L+3$ (14.2%)	4.756	0.051	260.7	^{1}MLCT/^{1}LLCT
S_{37}	$H-1 \rightarrow L+6$ (26.5%) $H \rightarrow L+11$ (18.6%) $H \rightarrow L+12$ (13.5%)	4.780	0.057	259.4	^{1}LLCT/^{1}MLCT
S_{39}	$H-2 \rightarrow L+4$ (46.9%) $H-3 \rightarrow L+4$ (14.8%) $H \rightarrow L+11$ (11.5%)	4.829	0.024	256.8	^{1}LLCT/^{1}MLCT
S_{40}	$H-1 \rightarrow L+6$ (20.5%) $H-7 \rightarrow L+1$ (18.9%) $H-11 \rightarrow L$ (15.2%)	4.840	0.054	256.2	^{1}LLCT/^{1}MLCT
S_{43}	$H-3 \rightarrow L+4$ (61.3%)	4.884	0.044	253.8	^{1}MLCT/^{1}LLCT
S_{44}	$H-4 \rightarrow L+2$ (45.7%) $H-1 \rightarrow L+5$ (19.3%)	4.893	0.027	253.4	^{1}LLCT/^{1}MLCT

2b

State	Major contribution (%)	E (eV)	*f*	λ_{cal} (nm)	Assignment
S_3	*H−1 → L* (87.5%)	3.131	0.033	396	^{1}ILCT/^{1}MLCT
S_{10}	*H−1 → L+1* (57.9%) *H−4 → L* (31.9%)	3.736	0.021	331.9	^{1}ILCT/^{1}MLCT
S_{13}	*H → L+7* (38.8%) *H → L+8* (38.3%)	3.950	0.028	313.9	^{1}LLCT
S_{14}	*H−1 → L+3* (39.7%) *H−2 → L+3* (13.7%)	3.970	0.039	312.3	^{1}LLCT/^{1}MLCT
S_{15}	*H−2 → L+3* (29.2%)	3.985	0.042	311.1	^{1}MLCT/^{1}ILCT
S_{16}	*H−1 → L+2* (39.6%) *H−2 → L+3* (16.6%)	4.010	0.030	309.2	^{1}LLCT/^{1}MLCT
S_{19}	*H → L+9* (69.5%)	4.090	0.032	303.2	^{1}LLCT
S_{23}	*H−4 → L+1* (28.7%) *H−7 → L* (20.3%)	4.190	0.092	295.9	^{1}ILCT/^{1}MLCT/^{1}LLCT
S_{25}	*H−8 → L* (64.6%) *H−9 → L* (12.3%)	4.261	0.077	291	^{1}MLCT/^{1}LLCT
S_{31}	*H−10 → L* (23.6%) *H−3 → L+3* (20.5%) *H−9 → L* (14.4%)	4.518	0.056	274.4	^{1}LLCT/^{1}MLCT/^{1}LMCT
S_{32}	*H−3 → L+3* (29.4%)	4.535	0.068	273.4	^{1}LLCT/^{1}LMCT/^{1}M
S_{33}	*H−1 → L+3* (22.2%) *H−7 → L* (12.8%)	4.577	0.087	270.9	^{1}LLCT/^{1}MLCT
S_{36}	*H−1 → L+3* (21.1%) *H−5 → L+1* (12.6%)	4.662	0.104	266	^{1}LLCT/^{1}MLCT
S_{46}	*H−2 → L+3* (13.9%) *H → L+10* (13.6%)	4.818	0.093	257.3	^{1}MLCT/^{1}LLCT

3a

State	Major contribution (%)	E (eV)	*f*	λ_{cal} (nm)	Assignment
S_5	*H−3 → L* (49.1%) *H−1 → L+1* (35.1%)	3.718	0.045	333.5	^{1}MLCT/^{1}ILCT
S_6	*H−2 → L+1* (98.2%)	3.825	0.010	324.1	^{1}MLCT
S_7	*H−1 → L+1* (47.3%) *H−3 → L* (23.2%)	3.907	0.240	317.3	^{1}ILCT/^{1}MLCT
S_8	*H−4 → L* (41.1%)	4.097	0.033	302.6	^{1}LLCT/^{1}MLCT/^{1}IL
S_9	*H → L+2* (36.8%) *H−5 → L* (35.5%)	4.133	0.062	300	^{1}LLCT/^{1}MLCT/^{1}ILCT
S_{12}	*H−5 → L+1* (45.8%) *H−7 → L* (20.7%)	4.405	0.072	281.5	^{1}ILCT/^{1}MLCT
S_{13}	*H−7 → L* (39.0%) *H−1 → L+2* (31.9%)	4.578	0.076	270.8	^{1}LLCT/^{1}MLCT/^{1}ILCT
S_{20}	*H−7 → L+1* (38.5%) *H → L+6* (12.7%)	4.952	0.110	250.4	^{1}LLCT/^{1}MLCT
S_{22}	*H−2 → L+6* (50.9%) *H−2 → L+5* (27.7%)	5.002	0.079	247.9	^{1}MLCT
S_{24}	*H−3 → L+2* (32.1%)	5.140	0.451	241.2	^{1}MLCT/^{1}LLCT

S_{25}	$H-1 \rightarrow L+6$ (37.4%) $H-1 \rightarrow L+5$ (28.5%)	5.151	0.057	240.7	^{1}MLCT/^{1}LLCT
S_{26}	$H-3 \rightarrow L+2$ (17.5%) $H-7 \rightarrow L+1$ (16.4%)	5.176	0.063	239.5	^{1}MLCT/^{1}LLCT
S_{28}	$H \rightarrow L+7$ (62.8%) $H-1 \rightarrow L+3$ (12.6%)	5.253	0.036	236	^{1}LLCT/^{1}MLCT
S_{32}	$H-1 \rightarrow L+4$ (48.2%) $H-1 \rightarrow L+3$ (12.0%)	5.353	0.058	231.6	^{1}LLCT/^{1}MLCT
S_{33}	$H-2 \rightarrow L+4$ (51.9%) $H-9 \rightarrow L+1$ (32.0%)	5.375	0.032	230.7	^{1}MLCT
S_{36}	$H-10 \rightarrow L$ (42.1%) $H-5 \rightarrow L+2$ (15.4%)	5.460	0.378	227.1	^{1}ILCT/^{1}MLCT
S_{37}	$H-1 \rightarrow L+5$ (37.7%) $H-1 \rightarrow L+6$ (22.9%)	5.474	0.034	226.5	^{1}LLCT^{1}MLCT

3b

State	Major contribution (%)	E (eV)	*f*	λ_{cal} (nm)	Assignment
S_4	$H \rightarrow L+1$ (52.4%) $H-3 \rightarrow L$ (27.0%)	3.836	0.023	323.3	^{1}LLCT/^{1}MLCT
S_5	$H \rightarrow L+1$ (33.5%) $H-3 \rightarrow L$ (31.6%)	3.845	0.026	322.4	^{1}LLCT/^{1}MLCT
S_7	$H-1 \rightarrow L+1$ (54.9%)	4.010	0.210	309.2	^{1}MLCT/^{1}LLCT/^{1}IL
S_{11}	$H-3 \rightarrow L+1$ (44.6%) $H-3 \rightarrow L$ (13.8%)	4.247	0.099	291.9	^{1}MLCT/ ^{1}LLCT
S_{17}	$H-2 \rightarrow L+3$ (23.9%) $H-5 \rightarrow L+1$ (22.7%)	4.503	0.062	275.4	^{1}MLCT/^{1}ILCT
S_{18}	$H-1 \rightarrow L+3$ (46.3%) $H-7 \rightarrow L$ (11.3%)	4.518	0.029	274.4	^{1}LLCT/^{1}MLCT
S_{20}	$H-7 \rightarrow L$ (32.7%) $H-1 \rightarrow L+5$ (19.8%)	4.635	0.034	267.5	^{1}ILCT/^{1}MLCT
S_{32}	$H-8 \rightarrow L$ (66.0%) $H-9 \rightarrow L$ (28.3%)	4.950	0.065	250.7	^{1}LLCT/^{1}MLCT
S_{35}	$H-6 \rightarrow L+2$ (34.2%)	5.040	0.060	246.0	^{1}LLCT/^{1}MLCT
S_{36}	$H-7 \rightarrow L+1$ (41.4%) $H-3 \rightarrow L+5$ (13.4%)	5.073	0.026	244.4	^{1}MLCT
S_{39}	$H-12 \rightarrow L$ (30.5%) $H-13 \rightarrow L$ (17.3%)	5.109	0.097	242.7	^{1}LLCT
S_{40}	$H-3 \rightarrow L+4$ (24.6%) $H-12 \rightarrow L$ (14.3%)	5.132	0.050	241.6	^{1}MLCT/^{1}LLCT
S_{43}	$H-2 \rightarrow L+10$ (16.7%) $H \rightarrow L+10$ (12.4%)	5.195	0.037	238.7	^{1}MLCT/^{1}LLCT

3c

State	Major contribution (%)	E (eV)	*f*	λ_{cal} (nm)	Assignment
S_4	*H−3 → L* (59.5%) *H−1 → L+1* (24.4%)	3.826	0.054	324.0	^{1}MLCT/^{1}LLCT
S_7	*H−1 → L+1* (56.5%) *H−3 → L* (15.7%)	4.002	0.205	309.8	^{1}ILCT/^{1}MLCT
S_9	*H−3 → L+1* (36.5%) *H−5 → L* (15.5%)	4.233	0.075	292.9	^{1}MLCT/^{1}LLCT
S_{15}	*H−5 → L+1* (38.9%)	4.503	0.088	275.3	^{1}ILCT/^{1}MLCT
S_{17}	*H−7 → L* (37.5%) *H−1 → L+4* (24.8%)	4.635	0.043	267.5	^{1}ILCT/^{1}MLCT
S_{27}	*H−7→ L+1* (47.2%) *H−3 → L+4* (21.8%)	5.066	0.044	244.7	^{1}ILCT/^{1}MLCT
S_{28}	*H−11 → L* (35.8%) *H−12 → L* (25.4%)	5.084	0.063	243.9	^{1}LLCT
S_{30}	*H−3 → L+3* (12.7%) *H−3 → L+4* (12.2%)	5.121	0.196	242.1	^{1}MLCT/^{1}LLCT
S_{31}	*H → L+8* (26.1%) *H−2 → L+8* (22.2%)	5.128	0.103	241.8	^{1}MLCT/^{1}LLCT
S_{32}	*H → L+5* (59.9%)	5.156	0.060	240.5	^{1}MLCT/^{1}LLCT
S_{33}	*H → L+8* (29.8%) *H−6 → L+4* (11.3%)	5.159	0.109	240.3	^{1}MLCT/^{1}LLCT
S_{37}	*H−3→ L+3* (40.6%) *H−3→ L+4* (30.5%)	5.283	0.081	234.7	^{1}MLCT/^{1}LLCT
S_{38}	*H−1 → L+5* (16.7%) *H−6 → L+2* (12.9%)	5.293	0.046	234.2	^{1}LLCT/^{1}MLCT
S_{39}	*H−6 → L+2* (26.5%) *H−1 → L+8* (18.9%) *H−1 → L+6* (15.3%)	5.297	0.105	234.0	^{1}LLCT/^{1}MLCT
S_{41}	*H−5 → L+2* (37.1%) *H−1→ L+5* (30.8%)	5.366	0.056	231.1	^{1}LLCT/^{1}MLCT
S_{42}	*H−5 → L+2* (34.5%) *H−9 → L+1* (22.9%)	5.374	0.035	230.7	^{1}LLCT/^{1}MLCT
S_{43}	*H→ L+5* (24.4%) *H−8→ L+2* (10.8%)	5.385	0.045	230.2	^{1}LLCT/^{1}MLCT
S_{44}	*H → L+6* (39.3%) *H → L+10* (13.2%)	5.397	0.067	229.7	^{1}LLCT/^{1}MLCT

4a

State	Major contribution (%)	E (eV)	*f*	λ_{cal} (nm)	Assignment
S_4	*H−3 → L* (51.5%) *H → L+1* (34.8%)	3.382	0.044	323.6	^{1}MLCT/^{1}ILCT
S_7	*H→ L+1* (49.6%) *H−3 → L* (24.9%)	3.998	0.216	310.1	^{1}MLCT/^{1}LLCT
S_8	*H−3 → L+1* (65.7%) *H−7 → L* (18.1%)	4.213	0.025	294.3	^{1}MLCT/^{1}ILCT
S_9	*H−4 → L* (48.5%)	4.265	0.058	290.7	^{1}LLCT

S_{11}	$H-5 \rightarrow L$ (61.7%) $H-4 \rightarrow L$ (28.0%)	4.426	0.022	280.1	^{1}ILCT/^{1}MLCT
S_{12}	$H-5 \rightarrow L+1$ (32.5%) $H-7 \rightarrow L$ (20.6%)	4.498	0.059	275.6	^{1}ILCT/^{1}MLCT/^{1}LLCT
S_{13}	$H-7 \rightarrow L$ (40.8%) $H-1 \rightarrow L+2$ (35.3%)	4.672	0.058	265.4	^{1}LLCT/^{1}MLCT
S_{14}	$H-2 \rightarrow L+2$ (89.8%)	4.790	0.020	258.8	^{1}MLCT/^{1}LLCT
S_{16}	$H-2 \rightarrow L+4$ (46.5%) $H-2 \rightarrow L+6$ (25.9%)	4.818	0.048	257.3	^{1}MLCT
S_{22}	$H-7 \rightarrow L+1$ (52.1%)	5.069	0.103	244.6	^{1}LLCT/^{1}MLCT
S_{25}	$H-3 \rightarrow L+2$ (40.8%)	5.201	0.500	238.4	^{1}MLCT
S_{26}	$H-7 \rightarrow L+1$ (23.2%) $H-3 \rightarrow L+2$ (14.9%) $H \rightarrow L+5$ (13.1%)	5.216	0.133	237.7	^{1}LLCT/^{1}MLCT
S_{29}	$H \rightarrow L+3$ (69.8%) $H \rightarrow L+5$ (21.9%)	5.324	0.107	232.9	^{1}LLCT/^{1}MLCT
S_{30}	$H-2 \rightarrow L+6$ (53.8%) $H-2 \rightarrow L+4$ (31.0%)	5.385	0.040	230.2	^{1}MLCT
S_{32}	$H-2 \rightarrow L+5$ (65.4%)	5.419	0.040	228.8	^{1}MLCT
S_{33}	$H \rightarrow L+5$ (50.1%) $H \rightarrow L+3$ (13.7%)	5.426	0.056	228.5	^{1}LLCT/^{1}MLCT
S_{36}	$H-10 \rightarrow L$ (48.9%) $H-5 \rightarrow L+2$ (12.1%)	5.555	0.291	223.2	^{1}ILCT/^{1}MLCT
S_{43}	$H \rightarrow L+7$ (24.1%) $H-5 \rightarrow L+2$ (22.5%)	5.810	0.136	213.4	^{1}ILCT/^{1}MLCT
S_{44}	$H-1 \rightarrow L+4$ (22.3%) $H-1 \rightarrow L+6$ (21.3%)	5.826	0.375	212.8	^{1}MLCT/^{1}LLCT
S_{49}	$H-7 \rightarrow L+3$ (53.9%) $H \rightarrow L+7$ (18.1%)	5.926	0.059	204.4	^{1}MLCT/^{1}ILCT

Table S4. Molecular orbital contribution (%) in the triplet state for all complexes.

1a		**Contribution (%)**				**Orbital interpretation (from high effect to minimum)**
Orbitals	**E (eV)**	**Pt**	**bzq**	**Me**	**P-(Ph)$_2$(C$_3$H$_5$)**	
HOMO-1	-5.406	69	18	9	4	d(Pt) + π(bzq)
HOMO	-5.275	33	63	1	3	π(bzq) + d(Pt)
LUMO	-1.807	4	94	1	1	π*(bzq)
1b		**Contribution (%)**				**Orbital interpretation (from high effect to minimum)**
Orbitals	**E (eV)**	**Pt**	**bzq**	**Me**	**S-(Me)$_2$**	
HOMO-1	-5.527	88	7	3	2	d(Pt)
HOMO	-5.387	28	69	-	3	π(bzq) + d(Pt)
LUMO	-1.651	4	94	1	1	π*(bzq)
2a		**Contribution (%)**				**Orbital interpretation (from high effect to minimum)**
Orbitals	**E (eV)**	**Pt**	**bzq**	**S-(Ph)**	**P-(Ph)$_3$**	
HOMO-1	-5.527	16	75	1	7	π(bzq) + d(Pt)
HOMO	-5.387	6	7	3	84	π(P-Ph$_3$)
LUMO	-1.651	2	95	3	-	π*(bzq)
2b		**Contribution (%)**				**Orbital interpretation (from high effect to minimum)**
Orbitals	**E (eV)**	**Pt**	**bzq**	**S-(py)**	**P-(Ph)$_3$**	
HOMO-1	-5.527	24	37	2	36	π(bzq) + π(P-Ph$_3$) + d(Pt)
HOMO	-5.387	9	8	3	81	π(P-Ph$_3$)
LUMO	-1.651	3	91	5	1	π*(bzq)
3a		**Contribution (%)**				**Orbital interpretation (from high effect to minimum)**
Orbitals	**E (eV)**	**Pt**	**bzq**	***p-Me*C$_6$H$_4$**	**S(Me)$_2$**	
HOMO-1	-5.527	25	5	66	4	d(Pt) + π(*p-Me*C$_6$H$_4$)
HOMO	-5.387	22	76	-	2	π(bzq) + d(Pt)
LUMO	-1.651	2	96	2	-	π*(bzq)
3b		**Contribution (%)**				**Orbital interpretation (from high effect to minimum)**
Orbitals	**E (eV)**	**Pt**	**bzq**	***p-Me*C$_6$H$_4$**	**P(Ph)$_2$(Me)**	
HOMO-1	-5.527	18	50	27	5	π(bzq) + π(*p-Me*C$_6$H$_4$) + d(Pt)
HOMO	-5.387	20	32	42	6	π(*p-Me*C$_6$H$_4$) + π(bzq) + d(Pt)
LUMO	-1.651	2	95	2	1	π*(bzq)
3c		**Contribution (%)**				**Orbital interpretation (from high effect to minimum)**
Orbitals	**E (eV)**	**Pt**	**bzq**	***p-Me*C$_6$H$_4$**	**P(Ph)(Me)$_2$**	
HOMO-1	-5.527	19	60	17	4	π(bzq) + d(Pt) + π(*p-Me*C$_6$H$_4$)
HOMO	-5.387	19	23	51	7	π(*p-Me*C$_6$H$_4$) + π(bzq) + d(Pt)
LUMO	-1.651	2	94	2	2	π*(bzq)
4a		**Contribution (%)**				**Orbital interpretation (from high effect to minimum)**
Orbitals	**E (eV)**	**Pt**	**bzq**	**Ph**	**S-(Me)$_2$**	
HOMO-1	-5.527	44	6	45	5	d(Pt) + π(Ph)
HOMO	-5.387	31	66	-	2	π(bzq) + d(Pt)
LUMO	-1.651	3	94	3	-	π*(bzq)

Table S5. Optical properties and Exciton generation fractions χ_T (%) of selected systems determined by TD-DFT level. All energetic values are in eV and the notations are defined as "p, v, g" respectively stands for phosphorescence, vertical, and gap.

Complex	ΔE_{gap}	$E_{T1\text{-}p}$ (eV)	$E_{T1\text{-}ver}$ (eV)	$E_{S1\text{-}ver}$ (eV)	$E_{S1\text{-}T1}$ (gap/ver)	E_g- $E_{S1\text{-}ver}$	E_g- $E_{T1\text{-}ver}$	δ_S/δ_T	χ_T(%)
1a	3.776	2.28	2.591	3.22	0.63	0.56	1.18	0.47	86.48
1b	3.736	2.35	2.568	3.20	0.63	0.53	1.17	0.46	86.79
2a	2.681	1.83	1.988	2.39	0.40	0.29	0.69	0.42	87.68
2b	3.265	1.84	2.569	2.95	0.38	0.32	0.70	0.45	86.89
3a	3.646	2.23	2.705	3.23	0.53	0.42	0.94	0.44	87.16
3b	3.717	2.22	2.850	3.35	0.50	0.37	0.87	0.42	87.63
3c	4.277	2.20	2.833	3.34	0.51	0.36	0.87	0.41	87.89
4a	3.857	2.23	2.852	3.36	0.51	0.50	1.01	0.49	85.85

Table S6. The xyz coordinates of the optimized structure of our eight complexes.

1a

Pt	0.38518	2.09012	6.84288
P	0.58265	2.27340	4.47287
N	2.32980	1.24559	7.42344
C	0.22079	2.14630	8.89056
C	-0.80807	2.62966	9.70215
H	-1.71783	3.03118	9.25143
C	-0.71729	2.61834	11.11195
H	-1.55180	3.00809	11.70251
C	0.40347	2.12016	11.75864
H	0.46321	2.10751	12.85000
C	1.48287	1.62322	10.99380
C	1.37468	1.65510	9.57328
C	2.67661	1.08618	11.59197
H	2.74564	1.06549	12.68333
C	3.70545	0.60438	10.83287
H	4.60229	0.19306	11.30323
C	3.63342	0.62700	9.39706
C	2.46925	1.16806	8.78502
C	3.31167	0.76181	6.65900
H	3.16894	0.82951	5.58216
C	4.48754	0.19711	7.18249
H	5.24927	-0.17612	6.49640
C	4.65424	0.13672	8.55548
H	5.56109	-0.28796	8.99440
C	-1.56858	2.75500	6.64992
H	-2.20629	2.20159	7.35895
H	-2.02009	2.61928	5.65132
H	-1.63554	3.82938	6.90481
C	-0.04168	3.97576	3.93579
H	-1.09687	4.00996	4.24229
H	0.50092	4.66285	4.60900
C	0.13014	4.39676	2.50790
H	1.16061	4.45424	2.13789
C	-0.87373	4.72839	1.68749
H	-1.91820	4.68965	2.01318
H	-0.68436	5.05468	0.66121
C	-0.39548	1.03893	3.49706
C	-0.53270	1.07970	2.09628
H	-0.04746	1.86715	1.51924
C	-1.29184	0.11280	1.43192
H	-1.39171	0.15762	0.34446
C	-1.92088	-0.90805	2.15301
H	-2.51287	-1.66314	1.62977
C	-1.78895	-0.95850	3.54306
H	-2.27715	-1.75216	4.11368
C	-1.03260	0.00924	4.21186
H	-0.93332	-0.02136	5.29978
C	2.27907	2.24177	3.70928
C	3.17976	3.27004	4.05001
H	2.86357	4.07575	4.71735
C	4.48745	3.26603	3.56027
H	5.16947	4.07483	3.83381
C	4.92528	2.22717	2.73081
H	5.94933	2.22211	2.34996
C	4.04492	1.19490	2.39730
H	4.37736	0.37677	1.75337
C	2.73097	1.20084	2.88110
H	2.05739	0.38608	2.61094

1b

Pt	1.93425	8.36869	2.87255
S	3.72222	9.30287	4.24491
C	0.38097	7.78515	1.72075
C	3.77687	8.38025	5.82471
H	4.63597	8.72317	6.42007
H	3.83658	7.29993	5.63376
H	2.84085	8.60834	6.35240
C	5.32821	8.80088	3.52394
H	6.14517	9.13163	4.18224
H	5.40446	9.30517	2.55102
H	5.35781	7.71250	3.37666
C	-1.93897	7.36911	0.08243
H	-2.82041	7.20130	-0.54180
C	0.54905	12.66749	2.74523
H	0.87625	13.62829	3.14582
C	-2.44564	9.82037	0.20007
H	-3.33098	9.66654	-0.42349
C	-1.63699	8.67553	0.52952
C	-2.13399	11.07506	0.64427
H	-2.76152	11.93105	0.38313
C	-1.11123	6.31596	0.44272
H	-1.34508	5.30490	0.09657
C	-0.58862	12.56128	1.96103
H	-1.18974	13.44285	1.72267
C	-0.16313	10.17996	1.80091
C	0.03100	6.51818	1.24901
H	0.64662	5.65305	1.50164
C	-0.48162	8.85968	1.34079
C	1.29544	11.51078	3.02901
H	2.19705	11.56324	3.64313
C	-0.97425	11.29739	1.46499
N	0.95827	10.30189	2.57598
C	2.67008	6.45273	3.01359
H	1.91904	5.78589	3.47565
H	2.89736	6.05322	2.00816
H	3.59467	6.36266	3.61397

2a

Pt	2.63927	4.63917	3.12572
N	1.07692	6.04716	3.49416
C	3.20179	5.31552	5.00534
C	4.27578	4.99934	5.84177
H	5.01324	4.25393	5.54224
C	4.45884	5.61481	7.10172
H	5.31973	5.32520	7.71124
C	3.57441	6.56977	7.57492
H	3.72273	7.04008	8.55026
C	2.46556	6.93912	6.78008
C	2.30387	6.30733	5.51460
C	1.18596	6.67897	4.70315
C	0.24202	7.64926	5.12932
C	-0.82942	7.94796	4.25967
H	-1.57556	8.68997	4.55628
C	-0.92096	7.29611	3.04122
H	-1.73485	7.50184	2.34467
C	0.05356	6.34620	2.68951
H	0.03597	5.80585	1.73965
P	4.37920	3.16496	2.83314
S	1.75411	4.19515	0.89485
C	4.33806	1.98780	1.39664
C	4.54964	2.48639	0.09806
C	4.09956	0.61718	1.57081
C	4.54279	1.62274	-0.99762
H	4.72038	3.55190	-0.05816
C	4.08557	-0.24438	0.46749
H	3.92495	0.20900	2.56655
C	4.31075	0.25431	-0.81607
H	4.71134	2.02375	-1.99988
H	3.89587	-1.30937	0.61998
H	4.30068	-0.41894	-1.67667
C	6.01640	4.00838	2.58718
C	6.15630	5.37088	2.89660
C	7.12448	3.31012	2.07033
C	7.38313	6.01648	2.71173
H	5.29819	5.92553	3.27798
C	8.34904	3.95776	1.89074
H	7.02835	2.25982	1.78798
C	8.48192	5.31252	2.21326
H	7.47417	7.07787	2.95433
H	9.19952	3.40237	1.48788
H	9.43876	5.81961	2.06648
C	4.59528	2.02277	4.28440
C	5.84991	1.58126	4.73362
C	3.43714	1.56449	4.93571
C	5.94240	0.69639	5.81275
H	6.76357	1.93459	4.25392
C	3.53267	0.67173	6.00622
H	2.45787	1.91454	4.60328
C	4.78575	0.23704	6.44886
H	6.92598	0.36734	6.15688
H	2.62325	0.32307	6.50123
H	4.86095	-0.45398	7.29191
C	1.50089	7.92296	7.19800
C	0.43582	8.26569	6.41331
H	1.63733	8.39984	8.17260
H	-0.28657	9.01458	6.74703
C	0.83091	2.66803	0.94283
C	0.56975	2.00379	-0.27356
C	0.30976	2.10818	2.12703
C	-0.18391	0.82922	-0.30187
H	0.96974	2.42037	-1.20079
C	-0.43590	0.92606	2.09322
H	0.48455	2.61769	3.07719
C	-0.68995	0.27728	0.88083
H	-0.37147	0.33573	-1.25981
H	-0.82854	0.51343	3.02729
H	-1.27613	-0.64452	0.85682

2b

Pt	3.47859	3.81722	12.30641
S	5.53419	4.34766	13.53092
P	2.11577	4.65095	14.02988
N	4.60132	3.04518	10.64625
N	4.97150	6.81602	12.60921
C	1.92843	3.19521	11.07181
C	3.82213	2.56018	9.65081
C	2.40193	2.62598	9.85481
C	1.55832	2.13183	8.84841
C	2.13567	1.57729	7.64616
H	1.46834	1.20154	6.88161
C	5.82105	6.07854	13.30812
C	1.17693	3.34038	14.93558
C	2.74780	6.94143	15.59464
H	2.16596	7.51683	14.89184
C	2.90401	5.57022	15.42804
C	1.30579	6.70530	12.34093
H	2.31577	6.62881	11.96353
C	4.36431	2.02226	8.47966
C	-0.85961	7.75164	12.28496
H	-1.53633	8.48394	11.86463
C	1.14195	2.03727	14.44531
H	1.65027	1.79383	13.52592
C	0.44088	7.65123	11.81080
H	0.78255	8.30300	11.01797
C	0.88228	5.85443	13.36354
C	-0.31440	2.73636	10.20992
H	-1.38363	2.79159	10.37324
C	-0.42478	5.96284	13.83306
H	-0.78670	5.30697	14.60979
C	0.16767	2.19558	9.04698
H	-0.50465	1.82138	8.28618
C	3.67166	4.86245	16.35686
H	3.82024	3.79925	16.23989
C	3.46769	1.52414	7.46731
H	3.88898	1.10748	6.56201
C	5.90803	3.01563	10.50945
H	6.47994	3.41490	11.33131
C	6.97637	6.63786	13.88591
H	7.64384	6.00833	14.45500
C	0.52829	3.61821	16.14424
H	0.56993	4.61173	16.56762
C	5.23166	8.11018	12.45344
H	4.50429	8.66667	11.87268
C	0.55171	3.22814	11.20454
H	0.09068	3.64188	12.08742
C	4.08791	6.88234	17.59056
H	4.54628	7.38977	18.42929
C	4.25321	5.51080	17.43060
H	4.84442	4.94711	18.13965
C	5.76276	1.99963	8.35776
H	6.21689	1.59073	7.46417
C	-0.19606	1.33292	16.31593
H	-0.72723	0.55638	16.85045
C	6.53791	2.49682	9.37227
H	7.61611	2.49899	9.31704
C	-0.15773	2.62648	16.82408
H	-0.65434	2.86030	17.75629
C	0.45698	1.04021	15.13098
H	0.44237	0.03442	14.73363
C	3.33899	7.59479	16.67140
H	3.20803	8.66270	16.78356
C	-1.29130	6.90441	13.29443
H	-2.30570	6.97113	13.66464
C	7.22962	7.97794	13.71319
H	8.11430	8.42513	14.14950
C	6.33536	8.75095	12.97259
H	6.49263	9.80733	12.80842

3a

Pt	1.94144	8.38413	2.86025
S	3.76459	9.35033	4.29778
C	0.39624	7.79258	1.68898
C	3.82881	8.42124	5.85238
H	4.64934	8.79939	6.46049
H	3.94790	7.36003	5.65099
H	2.88542	8.59360	6.36649
C	5.36563	8.91463	3.56912
H	6.16302	9.28535	4.21163
H	5.42026	9.40724	2.60041
H	5.43772	7.83829	3.43787
C	2.73185	6.51304	3.01353
C	3.68500	6.02351	2.11302
H	4.00780	6.64384	1.28458
C	4.23351	4.74770	2.22597
H	4.96572	4.42121	1.49570
C	3.85504	3.88604	3.24697
C	2.89981	4.35132	4.14919
H	2.56818	3.70480	4.95505
C	2.35558	5.62270	4.03333
H	1.60419	5.92341	4.75460
C	-1.89470	7.37549	0.04900
H	-2.76294	7.20679	-0.57455
C	0.48716	12.65150	2.75935
H	0.79444	13.60371	3.16536
C	-2.43646	9.80846	0.18828
H	-3.30689	9.64844	-0.43463
C	-1.60715	8.67025	0.51336
C	4.43799	2.49778	3.37656
H	5.17349	2.30396	2.59475
H	3.66191	1.73191	3.29936
H	4.93424	2.36156	4.34115
C	-2.14826	11.04214	0.64012
H	-2.77793	11.88541	0.38899
C	-1.06483	6.33755	0.39518
H	-1.28402	5.33859	0.03835
C	-0.63273	12.52674	1.97499
H	-1.24150	13.39112	1.74234
C	-0.17368	10.17846	1.79782
C	0.06739	6.53905	1.20467
H	0.68542	5.68754	1.44602
C	-0.47365	8.85396	1.31971
C	1.23981	11.50557	3.03094
H	2.12586	11.57094	3.64485
C	-0.99086	11.26838	1.47097
N	0.92684	10.31635	2.57173

3b

Pt	1.42646	3.70591	2.54026
P	0.51184	5.53548	3.88097
N	3.24645	4.67858	1.72555
C	2.20525	2.17464	1.40654
C	3.69261	5.90155	1.89963
C	1.75568	6.55215	4.80425
C	-2.43687	1.01973	3.91099
C	-3.61863	0.17653	4.33116
C	-2.18820	8.45420	2.72268
C	2.75852	8.63186	5.51996
C	-2.51822	1.92077	2.85754
C	-1.20742	0.90920	4.55862
C	3.68956	7.93807	6.27607
C	-1.01584	7.72134	0.76021
C	3.59786	0.31964	-0.25270
C	-1.96821	8.53458	1.35328
C	2.42069	-0.02050	0.36765
C	5.83668	3.27652	-0.52602
C	1.79496	7.94441	4.78988
C	4.86439	6.38550	1.31236
C	5.59014	5.53897	0.51294
C	2.70752	5.86337	5.56182
C	-1.41932	2.68379	2.46876
C	-0.48671	6.74423	2.91008
C	5.35107	2.03486	-0.70003
C	-1.45371	7.56715	3.49362
C	-0.17989	2.58931	3.10995
C	-0.28419	6.82830	1.53307
C	-0.11411	1.66830	4.16751
C	-0.60090	5.01542	5.25243
C	1.73179	0.89216	1.18510
C	3.66132	6.54900	6.29636
C	3.42084	2.50746	0.75135
C	4.12286	1.60950	-0.06934
C	5.13960	4.22845	0.30372
C	3.94973	3.83494	0.93257
H	0.80985	0.57055	1.64576
H	2.01060	-1.01311	0.22556
H	4.12020	-0.39088	-0.88012
H	5.87947	1.32751	-1.32600
H	6.75633	3.58489	-1.00557
H	6.50541	5.87343	0.04143
H	5.17511	7.40244	1.49943
H	3.11194	6.54772	2.53720
H	-1.54369	3.36732	1.63688
H	-3.45464	2.03378	2.32236
H	-4.53079	0.49474	3.82445
H	-3.45935	-0.87892	4.09308
H	-3.79430	0.24396	5.40764
H	-1.10031	0.21268	5.38371
H	0.82013	1.53116	4.69967
H	-0.07132	4.28349	5.86019
H	-0.87553	5.86351	5.87833
H	-1.48759	4.53797	4.84075
H	2.71119	4.78083	5.56929
H	4.38859	5.99852	6.87797
H	4.43758	8.47460	6.84453
H	2.77585	9.71350	5.49545
H	1.08027	8.50502	4.20557
H	-2.93549	9.08092	3.19082
H	-2.54411	9.22519	0.75158
H	-1.64255	7.52274	4.55663
H	0.43932	6.18287	1.05547
H	-0.84574	7.77021	-0.30681

3c

Pt	4.28093	7.96526	3.09049
P	6.04233	9.44269	3.88060
N	5.52881	6.29180	2.35007
C	2.82396	6.65191	2.46125
C	5.56960	11.16048	4.33487
C	3.33999	5.44054	1.92836
C	7.17677	9.78687	1.35337
C	3.13646	3.20191	0.92662
C	8.18494	10.04560	0.43588
C	6.83622	6.16908	2.32753
C	4.47205	3.05086	0.89352
C	1.44367	6.76368	2.47944
C	4.77000	5.27135	1.88447
C	2.90871	9.32841	3.72809
C	0.97328	11.23730	4.62945
C	7.45220	9.73019	2.72090
C	5.34166	4.09489	1.37804
C	0.61165	5.73787	1.99887
C	2.52482	4.40342	1.44627
C	1.46358	11.25862	3.32459
C	7.49620	5.03584	1.84717
C	2.39909	9.31641	5.03059
C	-0.04846	12.24909	5.09451
C	6.73915	3.99535	1.36942
C	1.13121	4.57287	1.48919
C	1.45879	10.24554	5.47111
C	6.80538	8.82485	5.43897
C	2.40068	10.33313	2.88930
C	9.48807	10.24089	0.87100
C	8.76602	9.93251	3.14478
C	9.77722	10.18153	2.22675
H	1.10267	12.01209	2.63216
H	2.73819	10.39275	1.86092
H	2.72889	8.55582	5.72929
H	1.09594	10.18616	6.49139
H	-0.96093	12.19782	4.49481
H	-0.32638	12.07920	6.13555
H	0.33552	13.26975	5.01553
H	5.16379	11.66617	3.46036
H	4.79590	11.13417	5.10048
H	6.44313	11.70434	4.69773
H	5.99709	8.67600	6.15612
H	7.29075	7.86314	5.27089
H	7.52321	9.52723	5.86361
H	6.16718	9.61926	1.00212
H	10.27615	10.43658	0.15604
H	9.01666	9.89692	4.19555
H	10.79108	10.33197	2.57323
H	7.95179	10.08731	-0.61958
H	0.98029	7.65681	2.87149
H	-0.46282	5.87174	2.03373
H	0.48125	3.78864	1.12329
H	2.49143	2.41369	0.56047
H	4.91873	2.14586	0.50337
H	7.21103	3.09987	0.98561
H	8.57532	5.00080	1.85578
H	7.41215	7.00318	2.69563

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Pt	4.73037	5.67967	7.64604
C	5.45962	2.57266	7.37149
H	4.57691	2.52085	6.75153
C	6.22061	1.42440	7.60765
H	5.92301	0.48407	7.16810
C	7.33589	1.53158	8.40110
H	7.95081	0.66481	8.60716
C	7.68126	2.77498	8.94927
C	8.83295	2.98230	9.79288
H	9.46844	2.13614	10.01827
C	9.10889	4.20226	10.28763
H	9.97516	4.34819	10.91973
C	8.27157	5.34401	9.99740
C	8.54622	6.62467	10.50660
H	9.41035	6.77933	11.13943
C	7.70930	7.66690	10.19194
H	7.91862	8.65503	10.58315
C	6.58213	7.48355	9.37104
H	5.95842	8.33799	9.15589
C	6.26595	6.24446	8.84335
C	7.14320	5.17841	9.18008
C	6.85653	3.86863	8.65564
C	3.92344	7.54737	7.55630
C	4.29080	8.47061	6.56469
H	5.04426	8.19833	5.83454
C	3.73194	9.74193	6.49147
H	4.04930	10.42300	5.71033
C	2.77878	10.14554	7.41593
H	2.34418	11.13564	7.36353
C	2.40135	9.25974	8.41533
H	1.66747	9.55978	9.15434
C	2.96509	7.99013	8.48153
H	2.65695	7.33319	9.28680
C	2.85398	5.72547	4.64543
H	2.03862	5.35970	4.02300
H	3.80038	5.57764	4.12921
H	2.72479	6.77867	4.87994
C	1.31323	5.14381	6.90544
H	1.23087	6.21410	7.07466
H	1.25808	4.61623	7.85552
H	0.52228	4.78966	6.24587
N	5.76068	3.74818	7.87216
S	2.92132	4.74741	6.16964