Electronic Supplementary Information

A Theoretical Study on Tuning Electronic Structures and Photophysical Properties of New Designed Platinum (Ⅱ) Complexes by Adding Substituents on Functionalized Ligands as Highly Efficient OLED Emitters

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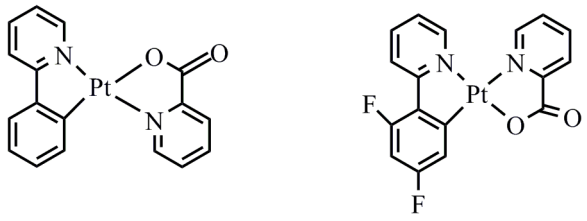
1. The comparison of the two configurations of Platinum (Ⅱ) complex 1.

1. The comparison of the two configurations of Platinum (Ⅱ) complex **1**.



trans-(ppy)Pt(pic) cis-(ppy)Pt(pic)

Figure S1. Two different chemical structures of complex **1**.

Table S1. Optimized geometries (Å) and energies (hartree) at the ground state (S_0) of trans-(ppy)Pt(pic) and cis-(ppy)Pt(pic), respectively

trans-(ppy)Pt(pic)				**cis-(ppy)Pt(pic)**			
Energy-1034.2268811				Energy=-1034.2213658			
C	-4.789032	1.175485	0.221262	C	4.971846	1.022653	0.115150
C	-2.474660	1.796831	0.385623	C	2.713808	1.826256	0.221661
C	2.972399	-3.121599	0.122673	C	-1.774701	3.737222	-0.184664
C	4.125477	-2.340119	0.231664	C	-3.130242	3.417668	-0.076979
C	1.744317	-2.482201	0.017622	C	-0.851113	2.702077	-0.170254
N	1.652066	-1.139214	0.013141	N	-1.198543	1.407993	-0.052090
C	4.019107	-0.953775	0.223267	C	-3.500758	2.083711	0.019311
C	2.760690	-0.350679	0.107598	C	-2.527892	1.074299	0.020815
C	2.466015	1.079893	0.036485	C	-2.782688	-0.359571	0.065053
C	3.463217	2.065571	0.017355	C	-4.058628	-0.943389	0.134546
C	1.084402	1.409800	-0.089139	C	-1.621056	-1.163770	0.007108
C	0.786059	2.760976	-0.314572	C	-1.763284	-2.556060	0.011734
C	3.122075	3.403316	-0.156576	C	-4.182250	-2.328446	0.141759
C	1.780287	3.743743	-0.341425	C	-3.034675	-3.129873	0.077909
Pt	-0.138224	-0.192579	-0.015835	Pt	0.106005	-0.189814	-0.016592
N	-2.074132	0.542132	0.105108	N	2.210021	0.590323	0.070450
O	-1.255293	-2.008124	-0.086939	O	1.191692	-1.910362	-0.053878
C	-2.535281	-1.861397	-0.224373	C	2.491960	-1.843158	-0.119947
O	-3.367323	-2.738535	-0.422162	O	3.249171	-2.798291	-0.221138
C	-4.374684	-0.129033	-0.030300	C	4.455945	-0.262297	-0.020508
C	-3.015048	-0.422202	-0.066472	C	3.074045	-0.442895	-0.031466
C	-3.817660	2.150883	0.449647	C	4.080250	2.088124	0.248049
H	-5.845306	1.426199	0.256467	H	6.044647	1.192654	0.127053
H	-1.691287	2.517131	0.573128	H	1.999299	2.632270	0.339551
H	3.016229	-4.205018	0.121576	H	-1.434079	4.762271	-0.280551
H	5.101312	-2.808888	0.321386	H	-3.885809	4.197847	-0.078719
H	0.800363	-3.011058	-0.061363	H	0.207124	2.899193	-0.270279
H	4.905390	-0.335151	0.305174	H	-4.546987	1.808292	0.085911
H	4.510124	1.792783	0.123867	H	-4.952334	-0.326208	0.182651
H	-0.235769	3.071435	-0.506755	H	-0.876895	-3.180287	-0.033202
H	3.893432	4.167909	-0.170732	H	-5.166438	-2.785352	0.195700
H	1.504496	4.781246	-0.515620	H	-3.135346	-4.212684	0.081346
H	-5.062206	-0.952337	-0.187833	H	5.078588	-1.144851	-0.112201
H	-4.085999	3.176813	0.678845	H	4.429179	3.108058	0.372883

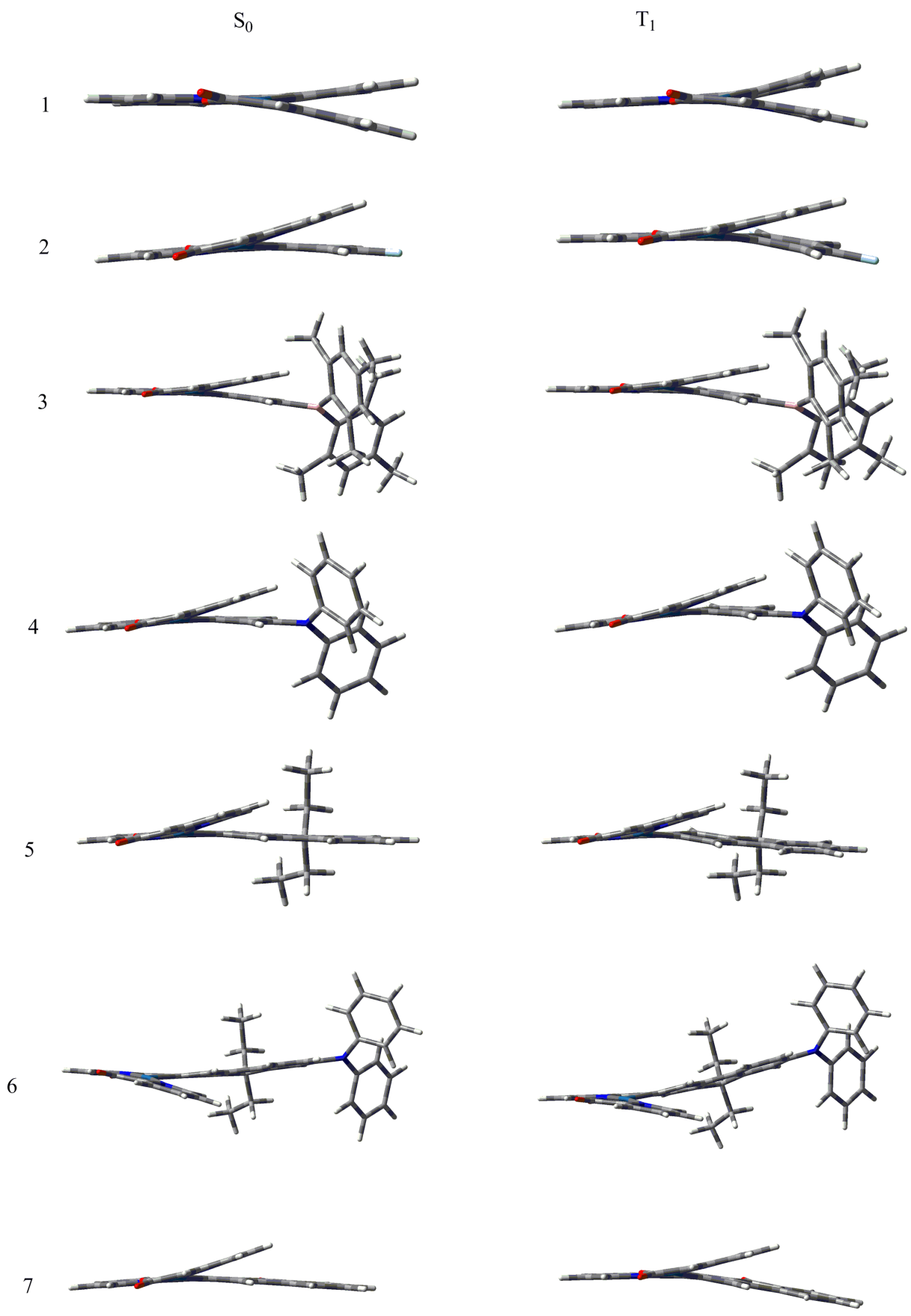


Figure S2. The optimized geometries of **1**-7 at their S_0 and $T_{1,opt}$ excited states, respectively

2. The energy-level Match of HOMO and LUMO among the typical Ir(Ⅲ) complexes and host materials in OLEDs.

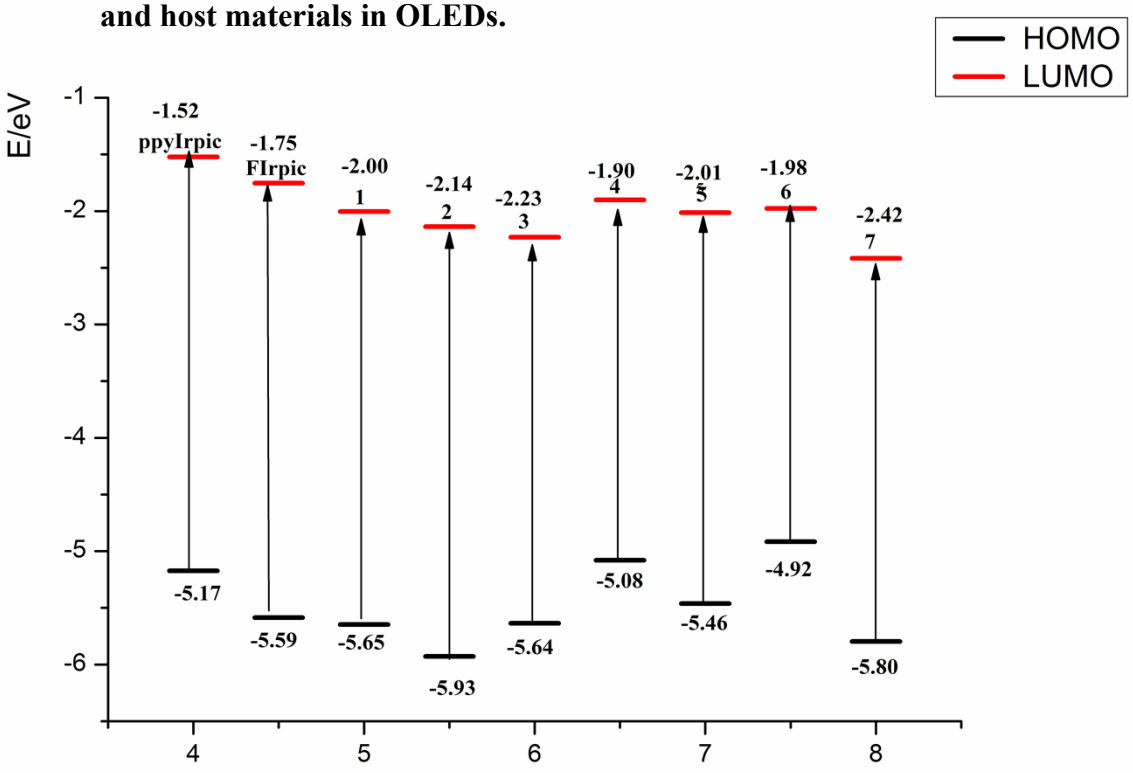


Figure S3. The molecular energy-level diagrams of host materials at the ground state optimization

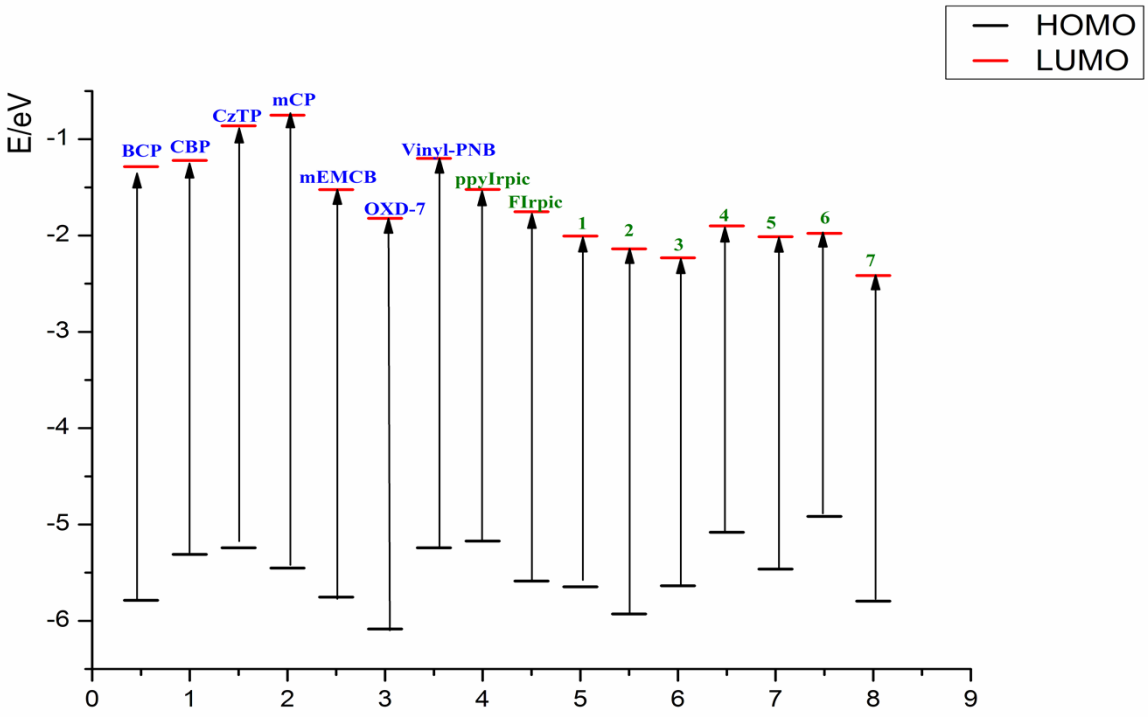


Figure S4. The molecular energy-level diagram match between host materials and guest material at their ground state optimizations

3. The analyses of MOs of complexes 1-7 at each S_0 geometric optimization.

Table S3. The analysis of the molecular orbitals at the S_0 geometry for **1** calculated by DFT/TDDFT approaches with GaussSum-2.2.5.

complex	Orbitals	Energy (eV)	MO compositions				
			pic	ppy	substituent	Pt (d%)	Composition contribution>15%
1	LUMO+4	-0.13	0.1645	0.3325	0.0000	0.5030(43.48)	d*(Pt)+π*(ppy)+π*(pic)
	LUMO+3	-1.07	0.4156	0.5692	0.0000	0.0152(1.48)	π*(ppy)+π*(pic)
	LUMO+2	-1.19	0.5745	0.4186	0.0000	0.0069(0.08)	π*(ppy)+π*(pic)
	LUMO+1	-1.57	0.4228	0.5359	0.0000	0.0412(3.87)	π*(ppy)+π*(pic)
	LUMO	-2.00	0.5358	0.4212	0.0000	0.0429(0.22)	π*(ppy)+π*(pic)
	HOMO	-5.65	0.1538	0.4563	0.0000	0.3900(38.31)	d(Pt)+π(ppy)+π(pic)
	HOMO-1	-6.27	0.1780	0.0710	0.0000	0.7510(58.67)	d(Pt)+π(pic)
	HOMO-2	-6.39	0.5120	0.1954	0.0000	0.2927(25.16)	d(Pt)+π(ppy)+π(pic)
	HOMO-3	-6.42	0.3370	0.5024	0.0000	0.1606(15.62)	d(Pt)+π(pic)+π(ppy)
	HOMO-4	-6.66	0.1017	0.3677	0.0000	0.5306(53.00)	d(Pt)+π(ppy)

Table S4. The analysis of the molecular orbitals at the S_0 geometry for **2** calculated by DFT/TDDFT approaches with GaussSum-2.2.5.

complex	Orbitals	Energy (eV)	MO compositions				
			pic	ppy	substituent	Pt (d%)	Composition contribution>15%
2	LUMO+4	-0.38	0.1536	0.3804	0.0071	0.4589(39.58)	d*(Pt)+π*(ppy)+π*(pic)
	LUMO+3	-1.13	0.1202	0.8586	0.0069	0.0143(1.20)	π*(ppy)
	LUMO+2	-1.30	0.8599	0.1304	0.0022	0.0075(0.27)	π*(pic)
	LUMO+1	-1.69	0.4005	0.5459	0.0109	0.0428(3.94)	π*(ppy)+π*(pic)
	LUMO	-2.14	0.5649	0.3849	0.0054	0.0448(0.30)	π*(ppy)+π*(pic)
	HOMO	-5.93	0.1798	0.4238	0.0058	0.3906(38.87)	π(ppy)+d(Pt)+π(pic)
	HOMO-1	-6.46	0.1830	0.5235	0.0482	0.2453(20.82)	π(ppy)+d(Pt)+π(pic)
	HOMO-2	-6.50	0.1841	0.2681	0.0255	0.5223(41.81)	π(ppy)+d(Pt)+π(pic)
	HOMO-3	-6.58	0.6477	0.0246	0.0007	0.3270(26.13)	d(Pt)+π(pic)
	HOMO-4	-6.82	0.1199	0.2472	0.0084	0.6245(62.41)	d(Pt)+π(ppy)

Table S5. The analysis of the molecular orbitals at the S_0 geometry for **3** calculated by DFT/TDDFT approaches with GaussSum-2.2.5.

complex	Orbitals	Energy (eV)	MO compositions				
			pic	ppy	substituent	Pt (d%)	Composition contribution>15%
3	LUMO+3	-1.04	0.8918	0.0505	0.0454	0.0123(0.88)	π*(pic)
	LUMO+2	-1.32	0.1943	0.6602	0.1139	0.0316(2.73)	π*(ppy)+π*(pic)
	LUMO+1	-1.75	0.7277	0.1242	0.1217	0.0264(1.17)	π*(pic)
	LUMO	-2.23	0.0925	0.6251	0.2525	0.0298(0.75)	π*(ppy)+π*(Substituent)
	HOMO	-5.64	0.1618	0.4274	0.0147	0.3960(39.44)	d(Pt)+π(ppy)+π(pic)
	HOMO-1	-6.08	0.0262	0.0707	0.8741	0.0291(2.13)	π(Substituent)
	HOMO-2	-6.21	0.0186	0.0448	0.8929	0.0438(3.6)	π(Substituent)
	HOMO-3	-6.25	0.0917	0.0815	0.5222	0.3047(23.97)	d(Pt)+π(Substituent)
	HOMO-4	-6.26	0.0983	0.0895	0.4279	0.3842(30.33)	d(Pt)+π(Substituent)
	HOMO-5	-6.36	0.6681	0.0176	0.0915	0.2228(18.12)	d(Pt)+π(pic)
	HOMO-6	-6.38	0.0465	0.0127	0.8944	0.0464(3.83)	π(Substituent)
	HOMO-7	-6.47	0.0932	0.3863	0.2100	0.3105(31.02)	d(Pt)+π(ppy)+(Substituent)
	HOMO-8	-6.67	0.0893	0.4411	0.0723	0.3972(39.64)	d(Pt)+π(ppy)

Table S6. The analysis of the molecular orbitals at the S_0 geometry for **4** calculated by DFT/TDDFT approaches with GaussSum-2.2.5

complex	Orbitals	Energy (eV)	MO compositions				
			pic	ppy	substituent	Pt (d%)	Composition contribution>15%
4	LUMO+5	-0.45	0.0018	0.1018	0.8857	0.0106(0.31)	π*(Substituent)
	LUMO+4	-0.53	0.0151	0.0746	0.8935	0.0167(1.27)	π*(Substituent)
	LUMO+3	-0.97	0.4603	0.5108	0.0116	0.0173(1.67)	π*(ppy)+π*(pic)
	LUMO+2	-1.10	0.5364	0.4344	0.0212	0.0080(0.18)	π*(ppy)+π*(pic)
	LUMO+1	-1.49	0.4224	0.4953	0.0445	0.0377(3.51)	π*(ppy)+π*(pic)
	LUMO	-1.90	0.5247	0.4110	0.0204	0.0439(0.26)	π*(ppy)+π*(pic)
	HOMO	-5.08	0.0037	0.3867	0.5907	0.0190(1.89)	π(ppy)+π(Substituent)
	HOMO-1	-5.65	0.1877	0.3257	0.0793	0.4073(40.44)	d(Pt)+π(ppy)+π(pic)
	HOMO-2	-6.19	0.1615	0.0548	0.0031	0.7806(61.16)	d(Pt)+π(pic)
	HOMO-3	-6.31	0.7595	0.0209	0.0017	0.2179(17.82)	d(Pt)+π(pic)
	HOMO-4	-6.46	0.1377	0.2249	0.0681	0.5692(56.88)	d(Pt)+π(ppy)

Table S7. The analysis of the molecular orbitals at the S_0 geometry for **5** calculated by DFT/TDDFT approaches with GaussSum-2.2.5

complex	Orbitals	Energy (eV)	MO compositions			
			pic	fpy	Pt(d%)	Composition contribution>15%
5	LUMO+5	-0.19	0.0012	0.9934	0.0054(0.49)	π^*(fpy)
	LUMO+4	-0.25	0.0194	0.9269	0.0538(1.98)	π^*(fpy)
	LUMO+3	-1.07	0.5554	0.4247	0.0199(1.90)	π^*(fpy)+π^*(pic)
	LUMO+2	-1.21	0.4623	0.5271	0.0105(0.45)	π^*(fpy)+π^*(pic)
	LUMO+1	-1.64	0.4906	0.4785	0.0309(2.97)	π^*(fpy)+π^*(pic)
	LUMO	-2.01	0.4383	0.5210	0.0408(0.23)	π^*(fpy)+π^*(pic)
	HOMO	-5.46	0.0748	0.6893	0.2358(13.49)	d(Pt)+π(fpy)
	HOMO-1	-5.94	0.1270	0.6805	0.1925(19.04)	d(Pt)+π(fpy)
	HOMO-2	-6.24	0.1381	0.0644	0.7975(62.38)	d(Pt)
	HOMO-3	-6.37	0.7786	0.0243	0.1971(16.35)	d(Pt)+π(pic)
	HOMO-4	-6.56	0.1383	0.1786	0.6831(68.26)	d(Pt)+π(fpy)
	HOMO-8	-7.19	0.0653	0.9170	0.0177(0.95)	π(fpy)

Table S8. The analysis of the molecular orbitals at the S_0 geometry for **6** calculated by DFT/TDDFT approaches with GaussSum-2.2.5

complex	Orbitals	Energy (eV)	MO compositions			
			pic	PhN_2-fpy	Pt (d%)	Composition contribution>15%
6	LUMO+6	-0.36	0.0027	0.9902	0.0071(0.11)	π^*(Ph2N-fpy)
	LUMO+5	-0.37	0.0012	0.9953	0.0034(0.05)	π^*(Ph2N-fpy)
	LUMO+3	-1.04	0.5330	0.4460	0.0210(1.98)	π^*(pic)+π^*(Ph2N-fpy)
	LUMO+2	-1.17	0.4869	0.5027	0.0104(0.46)	π^*(pic)+π^*(Ph2N-fpy)
	LUMO+1	-1.61	0.4838	0.4859	0.0303(2.90)	π^*(pic)+π^*(Ph2N-fpy)
	LUMO	-1.98	0.4427	0.5169	0.0404(0.22)	π^*(pic)+π^*(Ph2N-fpy)
	HOMO	-4.92	0.0018	0.9882	0.0100(0.99)	π(Ph2N-fpy)
	HOMO-1	-5.55	0.1254	0.5430	0.3316(33.01)	d(Pt)+π(Ph2N-fpy)
	HOMO-2	-6.10	0.0925	0.7928	0.1147(10.84)	π(Ph2N-fpy)
	HOMO-3	-6.21	0.1287	0.0870	0.7843(61.48)	d(Pt)
	HOMO-4	-6.34	0.7808	0.0257	0.1935(15.98)	d(Pt)+π(pic)
	HOMO-5	-6.53	0.1319	0.2001	0.6680(66.75)	d(Pt)+π(Ph2N-fpy)

Table S9. The analysis of the molecular orbitals at the S_0 geometry for **7** calculated by DFT/TDDFT approaches with GaussSum-2.2.5

complex	Orbitals	Energy (eV)	MO compositions			
			pic	CO-fpy	Pt(d%)	Composition contribution>15%
7	LUMO+6	-0.22	0.1647	0.3305	0.5048(44.80)	π*(CO-fpy)+π*(pic)+d*(Pt)
	LUMO+5	-0.34	0.0205	0.9292	0.0503(2.11)	π*(CO-fpy)
	LUMO+3	-1.45	0.4819	0.5076	0.0106(0.46)	π*(pic)+π*(CO-fpy)
	LUMO+2	-1.75	0.1680	0.8148	0.0172(1.66)	π*(pic)+π*(CO-fpy)
	LUMO+1	-1.84	0.6210	0.3586	0.0203(1.21)	π*(pic)+π*(CO-fpy)
	LUMO	-2.31	0.1418	0.8123	0.0459(1.40)	π*(CO-fpy)
	HOMO	-5.75	0.0930	0.6585	0.2485(24.73)	d(Pt)+π(CO-fpy)
	HOMO-1	-6.21	0.1739	0.6337	0.1923(18.65)	d(Pt)+π(CO-fpy)+π(pic)
	HOMO-2	-6.3	0.3741	0.0860	0.5400(42.54)	d(Pt)+π(pic)
	HOMO-3	-6.38	0.5464	0.0180	0.4356(34.77)	d(Pt)+π(pic)
	HOMO-4	-6.57	0.0129	0.9802	0.0068(0.63)	π(CO-fpy)
	HOMO-5	-6.68	0.1338	0.1855	0.6807(68.02)	d(Pt)+π(CO-fpy)

Note: [a]From **Table S3** to **Table S9**, "d" refers to the molecular orbitals with dominant d-orbital character, which took the contribution of d (Pt) orbitals over 10% into consideration

[b]The analyses of molecular fragment are calculated by GaussSum-2.2.5 and the atomic contribution are computed by Aomix.

4.The detailed absorption properties of each complex

Table S10. The abosrption properties of complex **1**

State	λcal (nm)	*f*	Ecal (eV)	Main configuration ψi→ψj		Excitation	orbitality interpretation	character of excitation
S1	426.2	0.019	2.91	81 → 82	0.69948	H→L (98%)	d(Pt)+π(ppy)+π(pic)→π*(ppy)+π*(pic)	MLCT+LLCT+ILCT
S2	372.3	0.012	3.33	81 → 83	0.67768	H→L+1 (92%)	d(Pt)+π(ppy)+π(pic)→π*(ppy)+π*(pic)	MLCT+LLCT+ILCT
S3	363.6	0.004	3.41	80 → 82	0.65059	H-1→L (85%)	d(Pt)+π(pic)→π*(ppy)+π*(pic)	MLCT+LLCT+ILCT
S4	355.7	0.002	3.49	78 → 82	0.30827	H-3→L (19%)	d(Pt)+π(pic)+π(ppy)→π*(ppy)+π*(pic)	MLCT+LLCT+ILCT
				79 → 82	0.54865	H-2→L (60%)	d(Pt)+π(ppy)+π(pic)→π*(ppy)+π*(pic)	MLCT+LLCT+ILCT
S5	329.7	0.012	3.76	79 → 82	0.15914	H-4→L (10%)	d(Pt)+π(ppy) →π*(ppy)+π*(pic)	MLCT+LLCT+ILCT
				81 → 84	0.60521	H→L+2 (73%)	d(Pt)+π(ppy)+π(pic)→π*(ppy)+π*(pic)	MLCT+LLCT+ILCT
S6	328	0.006	3.78	79 → 83	0.24439	H-2→L+1 (12%)	d(Pt)+π(ppy)+π(pic)→π*(ppy)+π*(pic)	MLCT+LLCT+ILCT
				80 → 83	0.63025	H-1→L+1 (79%)	d(Pt)+π(pic)→π*(ppy)+π*(pic)	MLCT+LLCT+ILCT
S7	326.5	0.136	3.80	78 → 82	0.49070	H-3→L (48%)	d(Pt)+π(pic)+π(ppy)→π*(ppy)+π*(pic)	MLCT+LLCT+ILCT
				79 → 82	-0.32556	H-2→L (21%)	d(Pt)+π(ppy)+π(pic)→π*(ppy)+π*(pic)	MLCT+LLCT+ILCT
				81 → 84	0.27580	H→L+2 (15%)	d(Pt)+π(ppy)+π(pic)→π*(ppy)+π*(pic)	MLCT+LLCT+ILCT
S8	320.4	0.006	3.87	81 → 85	0.64635	H→L+3 (84%)	d(Pt)+π(ppy)+π(pic)→π*(ppy)+π*(pic)	MLCT+LLCT+ILCT
S9	305.2	0.132	4.06	77 → 82	0.57090	H-4→L (65%)	d(Pt)+π(ppy)→π*(ppy)+π*(pic)	MLCT+LLCT+ILCT
				78 → 82	-0.23214	H-3→L (11%)	d(Pt)+π(pic)+π(ppy)→π*(ppy)+π*(pic)	MLCT+LLCT+ILCT
S10	310.3	0.009	4.11	79 → 83	0.38955	H-2→L+1 (30%)	d(Pt)+π(pic)+π(ppy)→π*(ppy)+π*(pic)	MLCT+LLCT+ILCT
				81 → 86	-0.36798	H→L+4 (27%)	d(Pt)+π(pic)+π(ppy)→d*(Pt)+π*(ppy)+π*(pic)	MLCT+LLCT+ILCT
S25	256.8	0.156	4.83	77 → 83	0.26193	H-4→L+1 (14%)	d(Pt)+π(ppy)→π*(ppy)+π*(pic)	MLCT+LLCT+ILCT
				78 → 85	0.44981	H-3→L+3 (40%)	d(Pt)+π(pic)+π(ppy)→π*(ppy)+π*(pic)	MLCT+LLCT+ILCT

Table S11. The abosrption properties of complex **2**

State	λcal (nm)	*f*	Ecal (eV)	Main configuration ψi→ψj		Excitation	orbitality interpretation	character of excitation
S1	406.2	0.017	3.05	89 → 90	0.69778	H→L (97%)	π(ppy)+d(Pt)+π(pic)→π*(ppy)+π*(pic)	MLCT+LLCT+ILCT
S2	359.6	0.033	3.45	86 → 90	-0.23894	H-3→L (11%)	d(Pt)+π(pic)→π*(ppy)+π*(pic)	MLCT+LLCT+ILCT
				87 → 90	0.40145	H-2→L (32%)	π(ppy)+d(Pt)+π(pic)→π*(ppy)+π*(pic)	MLCT+LLCT+ILCT
				88 → 90	-0.35329	H-1→L (25%)	π(ppy)+d(Pt)+π(pic)→π*(ppy)+π*(pic)	MLCT+LLCT+ILCT
				89 → 91	-0.32480	H→L+1 (21%)	π(ppy)+d(Pt)+π(pic)→π*(ppy)+π*(pic)	MLCT+LLCT+ILCT
S3	355.3	0.016	3.49	89 → 91	0.60454	H→L+1 (73%)	π(ppy)+d(Pt)+π(pic)→π*(ppy)+π*(pic)	MLCT+LLCT+ILCT
S4	349.9	0.003	3.84	86 → 90	0.58058	H-3→L (67%)	d(Pt)+π(pic)→π*(ppy)+π*(pic)	MLCT+LLCT+ILCT
				87 → 90	0.32830	H-2→L (22%)	π(ppy)+d(Pt)+π(pic)→π*(ppy)+π*(pic)	MLCT+LLCT+ILCT
S5	329.2	0.106	3.77	87 → 90	0.39509	H-2→L (31%)	π(ppy)+d(Pt)+π(pic)→π*(ppy)+π*(pic)	MLCT+LLCT+ILCT
				88 → 90	0.53684	H-1→L (58%)	π(ppy)+d(Pt)+π(pic)→π*(ppy)+π*(pic)	MLCT+LLCT+ILCT
S6	319.9	0.000	3.88	86 → 91	0.32368	H-3→L+1 (21%)	d(Pt)+π(pic)→π*(ppy)+π*(pic)	MLCT+LLCT+ILCT
				87 → 91	0.52415	H-2→L+1 (55%)	π(ppy)+d(Pt)+π(pic)→π*(ppy)+π*(pic)	MLCT+LLCT+ILCT
				88 → 91	-0.31749	H-1→L+1 (20%)	π(ppy)+d(Pt)+π(pic)→π*(ppy)+π*(pic)	MLCT+LLCT+ILCT
S7	315.1	0.006	3.94	85 → 90	0.27368	H-4→L (15%)	d(Pt)+π(ppy)→π*(ppy)+π*(pic)	MLCT+LLCT+ILCT
				89 → 92	0.61672	H→L+2 (76%)	π(ppy)+d(Pt)+π(pic)→π*(pic)	MLCT+LLCT+ILCT
S8	309.5	0.075	4.01	85 → 90	0.47028	H-4→L (44%)	d(Pt)+π(ppy)→π*(ppy)+π*(pic)	MLCT+LLCT+ILCT
				89 → 92	-0.28750	H→L+2 (17%)	π(ppy)+d(Pt)+π(pic)→π*(pic)	MLCT+LLCT+ILCT
				89 → 93	0.37058	H→L+3 (27%)	π(ppy)+d(Pt)+π(pic)→π*(ppy)	MLCT+LLCT+ILCT
S9	300.8	0.105	4.12	85 → 90	-0.35352	H-4→L (25%)	d(Pt)+π(ppy)→π*(ppy)+π*(pic)	MLCT+LLCT+ILCT
				89 → 93	0.53469	H→L+3 (57%)	π(ppy)+d(Pt)+π(pic)→π*(ppy)	MLCT+LLCT+ILCT
S10	297.7	0.000	4.16	86 → 91	0.39527	H-3→L+1 (31%)	d(Pt)+π(pic)→π*(ppy)+π*(pic)	MLCT+LLCT+ILCT
				88 → 91	0.29541	H-1→L+1 (17%)	π(ppy)+d(Pt)+π(pic)→π*(ppy)+π*(pic)	MLCT+LLCT+ILCT
				89 → 94	-0.30288	H→L+4 (18%)	π(ppy)+d(Pt)+π(pic)→d*(Pt)+π*(ppy)+π*(pic)	MLCT+LLCT+ILCT
S27	252.8	0.094	4.9	86 → 93	0.33849	H-3→L+3 (23%)	d(Pt)+π(pic)→π*(ppy)	MLCT+LLCT
				87 → 93	-0.33586	H-2→L+3 (23%)	π(ppy)+d(Pt)+π(pic)→π*(ppy)	MLCT+LLCT+ILCT
				88 → 93	-0.28764	H-1→L+3 (17%)	π(ppy)+d(Pt)+π(pic)→π*(ppy)	MLCT+LLCT+ILCT

Table S12. The abosrption properties of complex **3**

State	λcal (nm)	*f*	Ecal (eV)	Main configuration ψi→ψj		Excitation	orbitality interpretation	character of excitation
S1	451.3	0.037	2.75	148 →149	0.69128	H→L (96%)	d(Pt)+π(ppy)+π(pic)→π*(ppy)+π*(Substituent)	MLCT+LLCT+ILCT
S2	387.9	0.028	3.2	148 →150	0.67993	H→L+1 (92%)	d(Pt)+π(ppy)+π(pic)→π*(pic)	MLCT+LLCT+ILCT
S3	385.7	0.022	3.21	144 →149	-0.22117	H-4→L (10%)	d(Pt)+π(Substituent)→π*(ppy)+π*(Substituent)	MLCT+LLCT+ILCT
				145 →149	-0.28692	H-3→L (16%)	d(Pt)+π(Substituent)→π*(ppy)+π*(Substituent)	MLCT+LLCT+ILCT
				147 →149	0.54095	H-1→L (59%)	π(Substituent)→π*(ppy)+π*(Substituent)	LLCT+ILCT
S4	377.3	0.051	3.29	144 →149	0.40114	H-4→L (32%)	d(Pt)+π(Substituent)→π*(ppy)+π*(Substituent)	MLCT+LLCT+ILCT
				145 →149	0.32761	H-3→L (21%)	d(Pt)+π(Substituent)→π*(ppy)+π*(Substituent)	MLCT+LLCT+ILCT
				147 →149	0.40005	H-1→L (32%)	π(Substituent)→π*(ppy)+π*(Substituent)	LLCT+ILCT
S5	365.7	0.081	3.39	144 →149	-0.29105	H-4→L (17%)	d(Pt)+π(Substituent)→π*(ppy)+π*(Substituent)	MLCT+LLCT+ILCT
				146 →149	0.61235	H-2→L (75%)	π(Substituent)→π*(ppy)+π*(Substituent)	LLCT+ILCT
S6	360.3	0.001	3.44	143 →149	0.49820	H-5→L (50%)	d(Pt)+π(pic)→π*(ppy)+π*(Substituent)	MLCT+LLCT
				143 →150	-0.33227	H-5→L+1 (22%)	d(Pt)+π(pic)→π*(pic)	MLCT+ILCT
S7	357	0.078	3.47	144 →149	-0.38603	H-4→L (30%)	d(Pt)+π(Substituent)→π*(ppy)+π*(Substituent)	MLCT+LLCT+ILCT
				145 →149	0.51114	H-3→L (52%)	d(Pt)+π(Substituent)→π*(ppy)+π*(Substituent)	MLCT+LLCT+ILCT
				146 →149	-0.23301	H-2→L (11%)	π(Substituent)→π*(ppy)+π*(Substituent)	LLCT+ILCT
S8	344.8	0.008	3.6	142 →149	0.52215	H-6→L (55%)	π(Substituent)→π*(ppy)+π*(Substituent)	LLCT+ILCT
				148 →151	-0.42002	H→L+2 (35%)	d(Pt)+π(ppy)+π(pic)→π*(ppy)+π*(pic)	MLCT+LLCT+ILCT
S9	344.3	0.007	3.6	142 →149	0.40204	H-6→L (32%)	π(Substituent)→π*(ppy)+π*(Substituent)	LLCT+ILCT
				148 →151	0.53649	H→L+2 (58%)	d(Pt)+π(Substituent)→π*(ppy)+π*(pic)	MLCT+LLCT
S10	341.3	0.070	3.63	140 →149	0.22054	H-8→L (10%)	d(Pt)+π(ppy)→π*(ppy)+π*(Substituent)	MLCT+LLCT+ILCT
				141 →149	0.62345	H-7→L (78%)	d(Pt)+π(ppy)+π(Substituent)→π*(ppy)+π*(Substituent)	MLCT+LLCT+ILCT
S15	316.3	0.081	3.92	140 →149	0.34036	H-8→L (23%)	d(Pt)+π(ppy)→π*(ppy)+π*(Substituent)	MLCT+LLCT+ILCT
				148 →152	0.57244	H→L+3 (66%)	d(Pt)+π(ppy)+π(pic)→π*(pic)	MLCT+LLCT+ILCT
S22	299	0.090	4.15	140 →150	0.26455	H-8→L+1 (14%)	d(Pt)+π(ppy)→π*(pic)	MLCT+LLCT
				141 →150	0.50844	H-7→L+1 (52%)	d(Pt)+π(ppy)+π(Substituent)→π*(pic)	MLCT+LLCT

Table S13. The abosrption properties of complex **4**

State	λcal (nm)	*f*	Ecal (eV)	Main configuration ψi→ψj		Excitation	orbitality interpretation	character of excitation
S1	456.1	0.095	2.72	125 →126	0.68904	H→L (97%)	π(ppy)+π(Substituent)→π*(ppy)+π*(pic)	LLCT+ILCT
S2	409.1	0.026	3.03	124 →126	0.67092	H-1→L (90%)	d(Pt)+π(ppy)+π(pic)→π*(ppy)+π*(pic)	MLCT+LLCT+ILCT
S3	394.4	0.250	3.14	125 →127	0.66823	H→L+1 (89%)	π(ppy)+π(Substituent)→π*(ppy)+π*(pic)	LLCT+ILCT
S4	362.2	0.018	3.42	123 →126	-0.42731	H-2→L (37%)	d(Pt)+π(pic)→π*(ppy)+π*(pic)	MLCT+LLCT+ILCT
				124 →127	0.49735	H-1→L+1 (49%)	d(Pt)+π(ppy)+π(pic)→π*(ppy)+π*(pic)	MLCT+LLCT+ILCT
S5	359.1	0.008	3.45	123 →126	0.48931	H-2→L (48%)	d(Pt)+π(pic)→π*(ppy)+π*(pic)	MLCT+LLCT+ILCT
				124 →127	0.45719	H-1→L+1 (42%)	d(Pt)+π(ppy)+π(pic)→π*(ppy)+π*(pic)	MLCT+LLCT+ILCT
S6	354.7	0.064	3.5	125 →128	0.66311	H→L+2 (88%)	π(ppy)+π(Substituent)→π*(ppy)+π*(pic)	LLCT+ILCT
S7	353	0.002	3.51	122 →126	0.61204	H-3→L (75%)	d(Pt)+π(pic)→π*(ppy)+π*(pic)	MLCT+LLCT+ILCT
S8	342.1	0.015	3.62	125 →129	0.67474	H→L+3 (91%)	π(ppy)+π(Substituent))→π*(ppy)+π*(pic)	LLCT+ILCT
S9	325.9	0.002	3.8	122 →127	-0.22790	H-3→L+1 (10%)	d(Pt)+π(pic)→π*(ppy)+π*(pic)	MLCT+LLCT+ILCT
				123 →127	0.64884	H-2→L+1 (84%)	d(Pt)+π(pic)→π*(ppy)+π*(pic)	MLCT+LLCT+ILCT
S10	320.9	0.074	3.86	121 →126	0.45327	H-4→L (41%)	d(Pt)+π(ppy)→π*(ppy)+π*(pic)	MLCT+LLCT+ILCT
				124 →128	0.45773	H-1→L+2 (42%)	d(Pt)+π(ppy)+π(pic)→π*(ppy)+π*(pic)	MLCT+LLCT+ILCT
S14	309.7	0.124	4	124 →129	-0.38152	H-1→L+3 (29%)	d(Pt)+π(ppy)+π(pic)→π*(ppy)+π*(pic)	MLCT+LLCT+ILCT
				125 →130	0.31330	H→L+4 (20%)	π(ppy)+π(Substituent)→π*(Substituent)	LLCT+ILCT
				125 →131	0.47470	H→L+5 (45%)	π(ppy)+π(Substituent)→π*(Substituent)	LLCT+ILCT

Table S14. The abosrption properties of complex **5**

State	λcal (nm)	*f*	Ecal (eV)	Main configuration			orbitality interpretation	character of excitation
				ψi→ψj		Excitation		
S1	441.6	0.032	2.81	120 →121	0.67973	H→L (92%)	d(Pt)+π(fpy)→π*(fpy)+π*(pic)	MLCT+LLCT+ILCT
S2	387.4	0.056	3.2	120 →122	0.66640	H→L+1 (89%)	d(Pt)+π(fpy)→π*(fpy)+π*(pic)	MLCT+LLCT+ILCT
S3	367.8	0.073	3.37	118 →121	0.47876	H-2→L (46%)	d(Pt)→π*(fpy)+π*(pic)	MLCT
				119 →121	0.47359	H-1→L (45%)	d(Pt)+π(fpy)→π*(fpy)+π*(pic)	MLCT+LLCT+ILCT
S4	362.8	0.115	3.42	118 →121	0.48030	H-2→L (46%)	d(Pt)→π*(fpy)+π*(pic)	MLCT
				119 →121	-0.47496	H-1→L (45%)	d(Pt)+π(fpy)→π*(fpy)+π*(pic)	MLCT+LLCT+ILCT
S5	356.9	0.003	3.47	117 →121	0.60986	H-3→L (74%)	d(Pt)+π(pic)→π*(fpy)+π*(pic)	MLCT+LLCT+ILCT
				117 →122	0.25585	H-3→L+1 (13%)	d(Pt)+π(pic)→π*(fpy)+π*(pic)	MLCT+LLCT+ILCT
S6	341.6	0.032	3.63	120 →123	0.64260	H→L+2 (83%)	d(Pt)+π(fpy)→π*(fpy)+π*(pic)	MLCT+LLCT+ILCT
S7	333	0.007	3.72	118 →122	0.63829	H-2→L+1 (81%)	d(Pt)→π*(fpy)+π*(pic)	MLCT
S8	359.5	0.049	3.76	120 →124	0.61299	H→L+3 (75%)	d(Pt)+π(fpy)→π*(fpy)+π*(pic)	MLCT+LLCT+ILCT
S9	326.3	0.109	3.8	116 →121	-0.26117	H-4→L (14%)	d(Pt)+π(fpy)→π*(fpy)+π*(pic)	MLCT+LLCT+ILCT
				119 →122	0.57420	H→L+3 (66%)	d(Pt)+π(fpy)→π*(fpy)+π*(pic)	MLCT+LLCT+ILCT
				120 →124	0.22692	H→L+3 (10%)	d(Pt)+π(fpy)→π*(fpy)+π*(pic)	MLCT+LLCT+ILCT
S10	317.5	0.306	3.91	116 →121	0.57391	H-4→L (66%)	d(Pt)+π(fpy)→π*(fpy)+π*(pic)	MLCT+LLCT+ILCT
				119 →122	0.26410	H-1→L+1 (14%)	d(Pt)+π(fpy)→π*(fpy)+π*(pic)	MLCT+LLCT+ILCT

Table S15. The abosrption properties of complex **6**

State	λcal (nm)	*f*	Ecal (eV)	Main configuration ψi→ψj		Excitation	orbitality interpretation	character of excitation
S1	479.5	0.202	2.59	164 →165	0.68416	H→L (94%)	π(Ph2N-fpy)→π*(pic)+π*(Ph2N-fpy)	LLCT+ILCT
S2	425.4	0.080	2.91	163 →165	0.67122	H-1→L (90%)	d(Pt)+π(Ph2N-fpy)→π*(pic)+π*(Ph2N-fpy)	MLCT+LLCT+ILCT
S3	419.9	0.351	2.95	164 →166	0.68766	H→L+1 (95%)	π(Ph2N-fpy)→π*(pic)+π*(Ph2N-fpy)	LLCT+ILCT
S4	376.7	0.015	3.29	163 →166	0.65091	H-1→L+1 (85%)	d(Pt)+π(Ph2N-fpy)→π*(pic)+π*(Ph2N-fpy)	MLCT+LLCT+ILCT
S5	367.7	0.065	3.37	164 →167	0.65556	H→L+2 (86%)	π(Ph2N-fpy)→π*(pic)+π*(Ph2N-fpy)	LLCT+ILCT
S6	365.5	0.004	3.39	161 →165	0.63602	H-3→L (81%)	d(Pt)→π*(pic)+π*(Ph2N-fpy)	MLCT
S7	356.9	0.002	3.47	160 →165	0.60575	H-4→L (73%)	d(Pt)+π(pic)→π*(pic)+π*(Ph2N-fpy)	MLCT+LLCT+ILCT
				160 →166	0.25316	H-4→L+1 (13%)	d(Pt)+π(pic)→π*(pic)+π*(Ph2N-fpy)	MLCT+LLCT+ILCT
S8	353.6	0.018	3.51	164 →16	0.66754	H→L+3 (89%)	π(Ph2N-fpy)→π*(pic)+π*(Ph2N-fpy)	LLCT+ILCT
S9	339.7	0.158	3.65	162 →165	0.64031	H-2→L (82%)	π(Ph2N-fpy)→π*(pic)+π*(Ph2N-fpy)	LLCT+ILCT
S10	332.5	0.000	3.73	161 →166	0.63736	H-3→L+1 (81%)	d(Pt)→π*(pic)+π*(Ph2N-fpy)	MLCT
S14	317	0.158	3.91	159 →16	0.53172	H-5→L (57%)	d(Pt)+π(Ph2N-fpy)→π*(pic)+π*(Ph2N-fpy)	MLCT+LLCT+ILCT
				163 →16	-0.31029	H-1→L+3 (19%)	d(Pt)+π(Ph2N-fpy)→π*(pic)+π*(Ph2N-fpy)	MLCT+LLCT+ILCT
S15	309.8	0.188	4.00	164 →17	0.56069	H→L+5 (63%)	π(Ph2N-fpy)→π*(Ph2N-fpy)	ILCT
				164 →171	-0.40648	H→L+6 (33%)	π(Ph2N-fpy)→π*(Ph2N-fpy)	ILCT
S16	306.4	0.181	4.05	162 →166	0.51040	H-2→L+1 (52%)	π(Ph2N-fpy)→π*(pic)+π*(Ph2N-fpy)	LLCT+ILCT
				164 →171	-0.24316	H→L+6 (12%)	π(Ph2N-fpy)→π*(Ph2N-fpy)	ILCT
S17	305.1	0.113	4.06	160 →166	0.33006	H-4→L+1 (22%)	d(Pt)+π(pic)→π*(pic)+π*(Ph2N-fpy)	MLCT+LLCT+ILCT
				164 →170	0.27327	H→L+5 (15%)	π(Ph2N-fpy)→π*(Ph2N-fpy)	ILCT
				164 →171	0.37447	H→L+6(28%)	π(Ph2N-fpy)→π*(Ph2N-fpy)	ILCT

Table S16. The abosrption properties of complex **7**

State	λcal (nm)	*f*	Ecal (eV)	Main configuration ψi→ψj		Excitation	orbitality interpretation	character of excitation
S1	450.3	0.027	2.75	107 →108	0.69426	H→L (96%)	d(Pt)+π(CO-fpy)→π*(CO-fpy)	MLCT+ILCT
S2	401	0.006	3.09	106 →108	-0.38052	H-1→L (29%)	d(Pt)+π(CO-ppy)+π(pic)→π*(CO-fpy)	MLCT+LLCT+ILCT
				107 →109	0.56666	H→L+1 (64%)	d(Pt)+π(CO-fpy)→π*(pic)+π*(CO-fpy)	MLCT+LLCT+ILCT
S3	395.6	0.000	3.13	103 →108	0.58525	H-4→L (69%)	π(CO-fpy)→π*(CO-fpy)	ILCT
				103 →109	0.31056	H-4→L+1 (19%)	π(CO-fpy)→π*(pic)+π*(CO-fpy)	LLCT+ILCT
S4	377.6	0.010	3.28	106 →108	-0.32181	H-1→L (21%)	d(Pt)+π(CO-ppy)+π(pic)→π*(CO-fpy)	MLCT+LLCT+ILCT
				107 →109	-0.34585	H→L+1 (24%)	d(Pt)+π(CO-fpy)→π*(pic)+π*(CO-fpy)	MLCT+LLCT+ILCT
				107 →110	0.48492	H→L+2 (47%)	d(Pt)+π(CO-fpy)→π*(pic)+π*(CO-fpy)	MLCT+LLCT+ILCT
S5	369.8	0.007	3.35	105 →108	0.60640	H-2→L (74%)	d(Pt)+π(pic)→π*(CO-fpy)	MLCT+LLCT
S6	360.5	0.003	3.44	104 →108	0.54981	H-3→L (60%)	d(Pt)+π(pic)→π*(CO-fpy)	MLCT+LLCT
				104 →109	-0.31152	H-3→L+1 (19%)	d(Pt)+π(pic)→π*(pic)+π*(CO-fpy)	MLCT+LLCT+ILCT
				105 →109	0.22993	H-2→L+1 (11%)	d(Pt)+π(pic)→π*(pic)+π*(CO-fpy)	MLCT+LLCT+ILCT
S7	347.1	0.345	3.57	106 →108	0.42672	H-1→L (36%)	d(Pt)+π(CO-ppy)+π(pic)→π*(CO-fpy)	MLCT+LLCT+ILCT
				106 →109	-0.22997	H-1→L+1 (11%)	d(Pt)+π(CO-ppy)+π(pic)→π*(pic)+π*(CO-fpy)	MLCT+LLCT+ILCT
				107 →110	0.35164	H→L+2 (25%)	d(Pt)+π(CO-fpy)→π*(pic)+π*(CO-fpy)	MLCT+LLCT+ILCT
S8	333.6	0.029	3.73	102 →108	0.35202	H-5→L (25%)	d(Pt)+π(CO-fpy)→π*(CO-fpy)	MLCT+ILCT
				105 →109	0.40990	H-2→L+1 (34%)	d(Pt)+π(pic)→π*(pic)+π*(CO-fpy)	MLCT+LLCT+ILCT
				107 →111	0.23252	H→L+3 (11%)	d(Pt)+π(CO-fpy)→π*(pic)+π*(CO-fpy)	MLCT+LLCT+ILCT
S9	333.2	0.011	3.72	102 →108	0.32453	H-5→L (21%)	d(Pt)+π(CO-fpy)→π*(CO-fpy)	MLCT+ILCT
				105 →109	-0.25631	H-2→L+1 (13%)	d(Pt)+π(pic)→π*(pic)+π*(CO-fpy)	MLCT+LLCT+ILCT
				106 →109	-0.27690	H-1→L+1 (15%)	d(Pt)+π(CO-ppy)+π(pic)→π*(pic)+π*(CO-fpy)	MLCT+LLCT+ILCT
				107 →111	0.35728	H→L+3 (26%)	d(Pt)+π(CO-fpy)→π*(pic)+π*(CO-fpy)	MLCT+LLCT+ILCT
S10	328.6	0.047	3.77	102 →108	-0.13608	H-5→L (34%)	d(Pt)+π(CO-fpy)→π*(CO-fpy)	MLCT+ILCT
				106 →109	0.39305	H-1→L+1 (27%)	d(Pt)+π(CO-ppy)+π(pic)→π*(pic)+π*(CO-fpy)	MLCT+LLCT+ILCT
				107 →110	0.21739	H→L+3 (14%)	d(Pt)+π(CO-fpy)→π*(pic)+π*(CO-fpy)	MLCT+LLCT+ILCT
S11	322.7	0.118	3.84	106 →109	0.39305	H-1→L+1 (31%)	d(Pt)+π(CO-ppy)+π(pic)→π*(pic)+π*(CO-fpy)	MLCT+LLCT+ILCT
				107 →111	0.39929	H→L+3 (32%)	d(Pt)+π(CO-fpy)→π*(pic)+π*(CO-fpy)	MLCT+LLCT+ILCT
S20	293.8	0.149	4.22	101 →108	0.38340	H-6→L (29%)	π(pic)+π(CO-fpy)→π*(CO-fpy)	LLCT+ILCT
				102 →109	0.27808	H-5→L+1 (15%)	d(Pt)+π(CO-fpy)→π*(pic)+π*(CO-fpy)	MLCT+LLCT+ILCT
				106 →111	0.22824	H-1→L+3 (10%)	d(Pt)+π(CO-ppy)+π(pic)→π*(pic)+π*(CO-fpy)	MLCT+LLCT+ILCT

5. The relationship between the frontier molecular orbitals and the natural transition orbitals

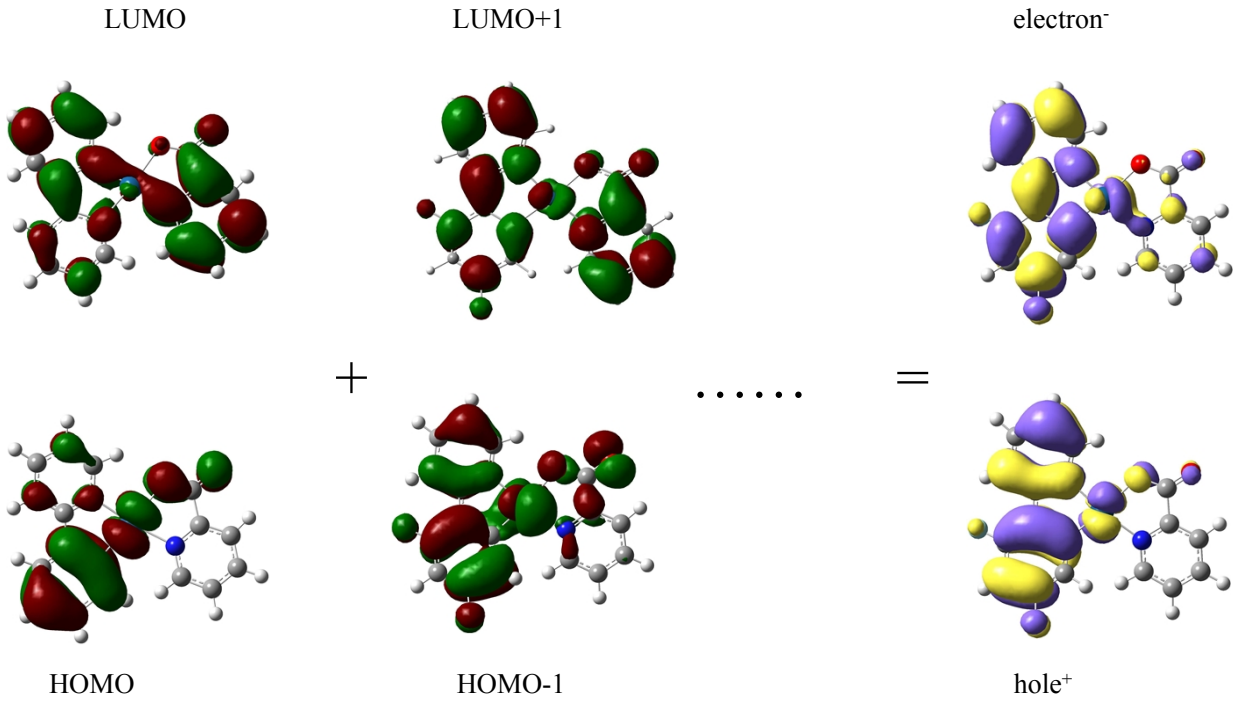


Figure S4. Comparison between the conventional analyses based on frontier molecular orbitals (FMO) and natural transition orbital (NTO) analysis of the $T_1 \rightarrow S_0$ transition of complex **2** at its T_1-state geometry. The description based on FMOs is displayed on the left-hand side and that based on NTOs on the right-hand side.

6. The calculation method of transition energies between 0-0 transition energy and $T_1 \rightarrow S_0$ vertical transition energy.

The 0-0 transition energies allow for the zero-point energies (zpe) of both S_0 and $T_{1,opt}$ at their respective optimized geometries. The vertical transition energies are achieved by the ΔSCF method, namely, it is the electronic-energy difference between the $T_{1,opt}$ and S_0 states at the $T_{1,opt}$ optimized geometries. The transition energy evaluated by the ΔSCF method is usually different from TDDFT. One of the reasons is that the former treats only a single configuration, DFT is a single-determinant theory; whilst the latter is a single-excitation theory, in which more than one configuration is considered in solving the eigenvalues of the excited states. Thus, the $T_{1,opt}$ excited state obtained from DFT calculations may differ from that obtained by TDDFT[1].

7. Cartesian coordinates of complexes 1-7 at their respective S_0 and $T_{1,opt}$ optimised geometries

Table S17. Cartesian coordinates of **1** at the S_0 optimized geometry.

C	-4.789032	1.175485	0.221262
C	-2.474660	1.796831	0.385623
C	2.972399	-3.121599	0.122673
C	4.125477	-2.340119	0.231664
C	1.744317	-2.482201	0.017622
N	1.652066	-1.139214	0.013141
C	4.019107	-0.953775	0.223267
C	2.760690	-0.350679	0.107598
C	2.466015	1.079893	0.036485
C	3.463217	2.065571	0.017355
C	1.084402	1.409800	-0.089139
C	0.786059	2.760976	-0.314572
C	3.122075	3.403316	-0.156576
C	1.780287	3.743743	-0.341425
Pt	-0.138224	-0.192579	-0.015835
N	-2.074132	0.542132	0.105108
O	-1.255293	-2.008124	-0.086939
C	-2.535281	-1.861397	-0.224373
O	-3.367323	-2.738535	-0.422162
C	-4.374684	-0.129033	-0.030300
C	-3.015048	-0.422202	-0.066472
C	-3.817660	2.150883	0.449647
H	-5.845306	1.426199	0.256467
H	-1.691287	2.517131	0.573128
H	3.016229	-4.205018	0.121576
H	5.101312	-2.808888	0.321386
H	0.800363	-3.011058	-0.061363
H	4.905390	-0.335151	0.305174
H	4.510124	1.792783	0.123867
H	-0.235769	3.071435	-0.506755
H	3.893432	4.167909	-0.170732
H	1.504496	4.781246	-0.515620
H	-5.062206	-0.952337	-0.187833
H	-4.085999	3.176813	0.678845

Table S18. Cartesian coordinates of **1** at the $T_{1,opt}$ optimized geometry.

C	4.801351	1.116344	-0.220772
C	2.495490	1.764758	-0.424105
C	-3.045289	-3.065347	-0.097656
C	-4.209594	-2.248560	-0.192683
C	-1.799136	-2.463647	-0.018474
N	-1.651561	-1.127223	-0.026205
C	-4.071077	-0.883243	-0.193451
C	-2.780914	-0.286033	-0.101490
C	-2.463449	1.079103	-0.046527
C	-3.410305	2.151682	-0.109783
C	-1.019784	1.395049	0.134497
C	-0.686347	2.725641	0.447028
C	-3.002590	3.436165	0.135107
C	-1.635318	3.737715	0.451651
Pt	0.129905	-0.199343	-0.009859
N	2.075218	0.518688	-0.123177
O	1.212763	-2.006095	0.104456
C	2.501453	-1.877159	0.252150
O	3.304434	-2.774132	0.470752
C	4.367504	-0.178906	0.047781
C	3.004695	-0.454730	0.075478
C	3.842550	2.099766	-0.476381
H	5.860676	1.353438	-0.249948
H	1.722968	2.490997	-0.636172
H	-3.114808	-4.147130	-0.091148
H	-5.192858	-2.703676	-0.257344
H	-0.877256	-3.031902	0.048244
H	-4.942554	-0.239520	-0.253187
H	-4.455270	1.944026	-0.319972
H	0.339119	2.977080	0.698749
H	-3.729006	4.244655	0.110603
H	-1.353338	4.759773	0.685170
H	5.044631	-1.006915	0.225008
H	4.126501	3.117927	-0.721169

Table S19. Cartesian coordinates of **2** at the S_0 optimized geometry.

C	-2.127006	-3.789823	0.046560
C	-3.400367	-3.232726	0.176628
C	-1.037055	-2.934543	-0.040669
N	-1.190399	-1.597813	-0.009420
C	-3.552969	-1.850374	0.207137
C	-2.424536	-1.023907	0.106600
C	-2.374578	0.436211	0.070590
C	-3.493372	1.278339	0.065027
C	-1.068835	1.010200	-0.052781
C	-0.981890	2.392574	-0.250741
C	-3.404409	2.653500	-0.087166
C	-2.130504	3.178519	-0.260040
F	-4.737688	0.759408	0.202720
F	-2.005647	4.507374	-0.445506
Pt	0.408324	-0.356241	-0.009211
N	2.189300	0.701652	0.138991
O	1.815658	-1.940619	-0.111882
C	2.369210	1.997602	0.457080
C	3.631421	2.576763	0.524403
C	4.754167	1.791532	0.260060
C	4.569737	0.442187	-0.026842
C	3.280895	-0.080184	-0.064066
C	3.052440	-1.575082	-0.255045
O	4.016708	-2.295158	-0.478674
H	-1.972428	-4.862622	0.016503
H	-4.275261	-3.871966	0.253620
H	-0.012881	-3.280002	-0.132114
H	-4.531721	-1.404523	0.304736
H	-0.039777	2.893082	-0.435610
H	-4.288913	3.278028	-0.089572
H	1.476122	2.565705	0.674893
H	3.720872	3.626347	0.783801
H	5.751231	2.220775	0.295858
H	5.388162	-0.244430	-0.211561

Table S20. Cartesian coordinates of **2** at the $T_{1,opt}$ optimized geometry.

C	2.181545	-3.759895	0.021717
C	3.481187	-3.184370	-0.099589
C	1.070145	-2.928467	0.072786
N	1.175674	-1.592719	0.016897
C	3.608857	-1.820828	-0.153584
C	2.452734	-0.979538	-0.085644
C	2.379207	0.416723	-0.076315
C	3.490504	1.327983	-0.152571
C	1.019868	1.006612	0.085955
C	0.925948	2.377186	0.350177
C	3.355247	2.666480	0.055347
C	2.056534	3.176816	0.338118
F	4.725042	0.836127	-0.410432
F	1.955096	4.496230	0.587499
Pt	-0.405551	-0.362887	-0.006274
N	-2.191268	0.687161	-0.154854
O	-1.792111	-1.944347	0.116665
C	-2.381671	1.982432	-0.478485
C	-3.647252	2.551786	-0.542861
C	-4.766132	1.759922	-0.274951
C	-4.571493	0.412398	0.015133
C	-3.279769	-0.101470	0.053421
C	-3.038260	-1.588221	0.253018
O	-3.988476	-2.325179	0.477465
H	2.042043	-4.833952	0.067956
H	4.358906	-3.820759	-0.145186
H	0.057603	-3.310151	0.153654
H	4.580971	-1.355609	-0.239612
H	-0.021451	2.849372	0.580330
H	4.213109	3.327745	0.018160
H	-1.492609	2.555393	-0.702476
H	-3.744415	3.599989	-0.805347
H	-5.765906	2.182245	-0.311304
H	-5.385866	-0.278497	0.202223

Table S21. Cartesian coordinates of **3** at the S_0 optimized geometry.

C	4.572367	-4.176689	0.433610
C	3.502821	-4.992692	0.809469
C	4.323760	-2.838022	0.157333
C	2.223384	-4.452783	0.889785
N	3.082667	-2.324802	0.240562
C	2.018008	-3.099790	0.596113
C	0.745642	-2.378525	0.587090
C	-0.490068	-2.993673	0.842033
C	0.831822	-1.000261	0.234210
C	-0.383234	-0.322830	0.090324
C	-1.668883	-2.269724	0.716099
C	-1.644433	-0.914408	0.324667
B	-2.963781	-0.078128	0.157969
C	-4.316025	-0.827544	-0.184195
C	-2.874348	1.497112	0.336155
C	-2.366267	2.067867	1.534820
C	-3.263041	2.382703	-0.705725
C	-3.130555	3.765747	-0.540725
C	-2.647442	4.329527	0.642916
C	-2.273959	3.458881	1.669631
C	-3.784960	1.877330	-2.035982
C	-2.575447	5.828751	0.820327
C	-1.926735	1.223371	2.718731
C	-5.474340	-0.685056	0.629411
C	-4.405671	-1.680712	-1.317898
C	-5.605637	-2.339410	-1.610645
C	-6.736653	-2.213885	-0.803059
C	-6.643632	-1.385211	0.318303
C	-3.243608	-1.904069	-2.270082
C	-8.027092	-2.921758	-1.143003
C	-5.484398	0.181852	1.872907
Pt	2.720803	-0.352641	-0.051071
N	2.621123	1.711040	-0.255893
C	1.585409	2.530916	0.006348
C	1.659539	3.906658	-0.181317
C	2.848581	4.464607	-0.650920
C	3.931396	3.621654	-0.885116
C	3.796756	2.254311	-0.666992
C	4.994835	1.323467	-0.818127
O	4.762718	0.101015	-0.454767
O	6.053782	1.788862	-1.221660

H	5.583027	-4.561963	0.356515
H	3.664636	-6.042440	1.036975
H	5.096734	-2.134081	-0.132620
H	1.382407	-5.073149	1.177665
H	-0.535847	-4.042929	1.123783
H	-0.385413	0.708637	-0.243093
H	-2.622289	-2.754775	0.907278
H	-3.424302	4.421925	-1.358329
H	-1.908156	3.872305	2.608390
H	-3.006478	1.351357	-2.603844
H	-4.616589	1.178550	-1.909119
H	-4.131201	2.708664	-2.658423
H	-1.837875	6.109826	1.580071
H	-2.311252	6.333036	-0.116123
H	-3.543083	6.236894	1.142200
H	-2.551974	0.337011	2.859011
H	-0.897622	0.863795	2.600701
H	-1.968661	1.808247	3.643850
H	-5.655671	-2.970297	-2.496672
H	-7.510522	-1.273732	0.967532
H	-3.610053	-2.211221	-3.255530
H	-2.629988	-1.009573	-2.408792
H	-2.571885	-2.691066	-1.907716
H	-7.854969	-3.767936	-1.816471
H	-8.526353	-3.299727	-0.243545
H	-8.733208	-2.244356	-1.642133
H	-4.797003	-0.196108	2.640401
H	-5.187063	1.211931	1.655336
H	-6.483590	0.205382	2.319474
H	0.685014	2.069888	0.384142
H	0.788301	4.513381	0.041265
H	2.932371	5.535027	-0.815750
H	4.898977	3.975161	-1.222973

Table S22. Cartesian coordinates of **3** at the $T_{1,opt}$ optimized geometry.

C	4.610629	-4.191905	0.168090
C	3.533844	-5.058702	0.469359
C	4.357544	-2.836839	0.012250
C	2.261965	-4.545722	0.592731
N	3.118906	-2.329925	0.136636
C	2.032470	-3.154615	0.420483
C	0.801074	-2.470802	0.478461
C	-0.463034	-3.061958	0.753322
C	0.861854	-1.010497	0.185928
C	-0.349166	-0.330422	0.034141
C	-1.608749	-2.318053	0.643483
C	-1.614887	-0.908497	0.259072
B	-2.918022	-0.089973	0.111295
C	-4.307306	-0.839875	-0.084398
C	-2.814535	1.501591	0.155524
C	-2.294602	2.171396	1.296233
C	-3.229291	2.303769	-0.942608
C	-3.117008	3.696718	-0.886830
C	-2.621655	4.356997	0.241222
C	-2.215821	3.571521	1.322318
C	-3.765744	1.686227	-2.217868
C	-2.570576	5.866571	0.300686
C	-1.828557	1.426383	2.535493
C	-5.423186	-0.599056	0.766279
C	-4.483246	-1.780381	-1.138363
C	-5.712465	-2.427879	-1.315110
C	-6.800075	-2.198330	-0.472321
C	-6.627561	-1.280875	0.567231
C	-3.381968	-2.113368	-2.128458
C	-8.125159	-2.889756	-0.691979
C	-5.349587	0.356761	1.939875
Pt	2.713563	-0.356250	0.007753
N	2.582630	1.726723	-0.075079
C	1.543011	2.522924	0.240178
C	1.604298	3.906619	0.118682
C	2.784545	4.498421	-0.331349
C	3.872269	3.677984	-0.619052
C	3.748774	2.300729	-0.472377
C	4.943614	1.387900	-0.693630
O	4.718039	0.136070	-0.405167
O	6.001177	1.866503	-1.076708

H	5.623386	-4.562619	0.059772
H	3.708726	-6.122623	0.598308
H	5.134416	-2.114336	-0.213924
H	1.422132	-5.195123	0.814126
H	-0.526144	-4.110347	1.032756
H	-0.335958	0.705552	-0.284118
H	-2.567707	-2.790283	0.841525
H	-3.435189	4.283794	-1.746987
H	-1.844942	4.060403	2.222524
H	-2.996547	1.097277	-2.733972
H	-4.606164	1.013506	-2.022206
H	-4.104230	2.459939	-2.914767
H	-1.905469	6.216432	1.097948
H	-2.223350	6.296742	-0.646144
H	-3.564242	6.290710	0.498243
H	-2.458390	0.561656	2.762036
H	-0.806368	1.042162	2.426682
H	-1.839285	2.086850	3.409365
H	-5.821660	-3.129747	-2.140472
H	-7.458035	-1.086285	1.244080
H	-3.800357	-2.589415	-3.021815
H	-2.824910	-1.229087	-2.451546
H	-2.646848	-2.809673	-1.704781
H	-8.009345	-3.795061	-1.297372
H	-8.592185	-3.174177	0.258022
H	-8.835075	-2.234927	-1.215491
H	-4.663932	-0.007044	2.716017
H	-4.998545	1.348350	1.640639
H	-6.332712	0.472450	2.407833
H	0.648206	2.038195	0.601347
H	0.727327	4.491098	0.374648
H	2.858140	5.576367	-0.441723
H	4.832672	4.058531	-0.947881

Table S23. Cartesian coordinates of **4** at the S_0 optimized geometry.

C	-4.013765	-3.952515	-0.294627
C	-3.728430	-2.614676	-0.058221
C	-2.965695	-4.804705	-0.656490
C	-1.674953	-4.301380	-0.761354
C	-1.430072	-2.944337	-0.507268
C	-0.145908	-2.258035	-0.527672
C	1.079486	-2.900762	-0.758004
C	-0.191669	-0.866945	-0.213699
C	1.030472	-0.211331	-0.059248
C	2.276995	-2.205674	-0.666653
C	2.263675	-0.848880	-0.294663
N	3.474798	-0.129106	-0.156737
C	4.635229	-0.763744	0.373736
C	3.531740	1.252117	-0.494652
C	4.174666	2.168026	0.353326
C	2.948612	1.719251	-1.684987
C	2.994217	3.075497	-2.005654
C	3.636918	3.984582	-1.159787
C	4.231148	3.519834	0.015852
C	5.889700	-0.554293	-0.220353
C	7.027019	-1.163313	0.307800
C	6.930775	-2.000847	1.421537
C	5.682292	-2.216012	2.010042
C	4.542126	-1.597329	1.499476
Pt	-2.060535	-0.162410	0.049358
N	-2.475420	-2.134692	-0.164522
H	-5.032690	-4.310661	-0.199060
H	-4.481383	-1.883719	0.217164
H	-3.155469	-5.855954	-0.854258
H	-0.852633	-4.951276	-1.038542
H	1.108451	-3.955748	-1.019232
H	1.062271	0.815564	0.282144
H	3.218886	-2.704221	-0.867071
H	4.624995	1.814475	1.275280
H	2.463251	1.013705	-2.351928
H	2.543406	3.418178	-2.933552
H	3.682165	5.038656	-1.418835
H	4.732440	4.214420	0.684789
H	5.965544	0.085822	-1.093804
H	7.991065	-0.991462	-0.163671
H	7.817949	-2.479229	1.826532

H	5.594074	-2.858108	2.882463
H	3.575642	-1.754902	1.967589
N	-1.894444	1.902241	0.147872
C	-0.839417	2.670789	-0.183726
C	-0.865189	4.056218	-0.069229
C	-2.024466	4.677376	0.396554
C	-3.128786	3.885110	0.697875
C	-3.043391	2.504282	0.550310
C	-4.268636	1.620857	0.763437
O	-4.084133	0.377399	0.448230
O	-5.303822	2.140366	1.163081
H	0.033550	2.156953	-0.559591
H	0.017779	4.623185	-0.344936
H	-2.069680	5.757253	0.505301
H	-4.076922	4.288876	1.034597

Table S24. Cartesian coordinates of **4** at the $T_{1,opt}$ optimized geometry.

C	-3.903817	-4.018745	-0.227524
C	-3.659413	-2.666859	-0.026146
C	-2.825820	-4.868831	-0.595216
C	-1.567811	-4.334580	-0.737801
C	-1.343362	-2.944797	-0.521871
C	-0.124447	-2.250081	-0.588489
C	1.145972	-2.853787	-0.900105
C	-0.185535	-0.808392	-0.251609
C	1.014796	-0.152503	-0.075843
C	2.303045	-2.144825	-0.754993
C	2.270978	-0.779206	-0.302704
N	3.474848	-0.076736	-0.141182
C	4.615816	-0.733630	0.393193
C	3.548206	1.307262	-0.461922
C	4.209633	2.204205	0.393861
C	2.947262	1.790566	-1.637521
C	3.006630	3.148468	-1.943657
C	3.667852	4.040055	-1.092748
C	4.270015	3.558629	0.073113
C	5.895307	-0.481833	-0.133605
C	7.004652	-1.140286	0.389072
C	6.858888	-2.061563	1.431361
C	5.587848	-2.314690	1.952899
C	4.470509	-1.655153	1.444969
Pt	-2.057210	-0.170944	0.026927
N	-2.435295	-2.133999	-0.167516
H	-4.910276	-4.402566	-0.105449
H	-4.439024	-1.964642	0.250914
H	-2.995328	-5.928862	-0.757954
H	-0.728999	-4.966340	-1.011018
H	1.189154	-3.881414	-1.248159
H	1.032315	0.869739	0.283122
H	3.258722	-2.595440	-1.002707
H	4.662338	1.835792	1.308530
H	2.447768	1.095030	-2.303941
H	2.548505	3.507711	-2.861210
H	3.717598	5.096911	-1.338420
H	4.780550	4.242637	0.745414
H	6.008073	0.219145	-0.954206
H	7.987737	-0.942134	-0.029083
H	7.727654	-2.575131	1.832621

H	5.463862	-3.019691	2.770209
H	3.485557	-1.832925	1.863928
N	-1.940845	1.897863	0.131484
C	-0.910350	2.698675	-0.208125
C	-0.969387	4.080837	-0.082157
C	-2.139481	4.672031	0.399705
C	-3.218640	3.848808	0.707801
C	-3.100064	2.471233	0.552592
C	-4.295940	1.557250	0.779369
O	-4.080505	0.317723	0.462861
O	-5.342592	2.044787	1.191471
H	-0.030620	2.208143	-0.599995
H	-0.104957	4.673132	-0.363900
H	-2.211056	5.749804	0.514062
H	-4.173448	4.225202	1.057369

Table S25. Cartesian coordinates of **5** at the S_0 optimized geometry.

C	-2.253209	4.508458	0.043836
C	-0.925087	4.916875	0.195111
C	-2.522317	3.149579	-0.048343
N	-1.536278	2.234601	-0.000573
C	0.086220	3.964510	0.239195
C	-0.229190	2.602763	0.134961
C	0.700595	1.477684	0.112945
C	2.097882	1.648293	0.131942
C	0.093140	0.190297	-0.010390
C	0.955470	-0.900318	-0.179699
C	2.926042	0.545689	-0.011086
C	2.343007	-0.730132	-0.166664
Pt	-1.924211	0.247942	-0.005033
H	-3.068007	5.222500	0.000476
H	-0.680067	5.972096	0.276366
H	-3.522841	2.745011	-0.158762
H	1.120266	4.268984	0.352774
H	2.523152	2.639938	0.255875
H	0.559324	-1.896839	-0.345618
C	3.417532	-1.723097	-0.264948
C	4.653870	-1.055298	-0.154971
C	3.368623	-3.110736	-0.422493
C	4.565511	-3.828778	-0.463236
C	5.842811	-1.776758	-0.197551
C	5.793828	-3.168139	-0.348933
C	4.454192	0.458343	-0.039685
C	5.114732	1.048367	1.235654
C	4.675104	0.411098	2.558513
C	5.063785	1.107730	-1.326288
C	4.914246	2.624045	-1.496001
H	2.416589	-3.628038	-0.511826
H	4.543515	-4.908610	-0.583896
H	6.803930	-1.274752	-0.113271
H	6.717863	-3.739367	-0.378975
H	6.204810	0.955454	1.129354
H	4.906329	2.125018	1.271395
H	5.185692	0.890485	3.401523
H	3.596477	0.519905	2.714426
H	4.911796	-0.657615	2.586611
H	6.132388	0.854068	-1.341863
H	4.619661	0.608404	-2.196173

H	5.419212	2.943306	-2.415047
H	3.864130	2.920504	-1.582845
H	5.362305	3.184440	-0.668020
C	-1.865143	-2.808867	0.479572
C	-2.436446	-4.074621	0.548204
C	-3.793082	-4.224119	0.257755
C	-3.906954	-1.848067	-0.093593
C	-4.534618	-3.089278	-0.056746
N	-2.574842	-1.717199	0.136389
O	-4.032847	0.516271	-0.166884
C	-4.716335	-0.574398	-0.315640
O	-5.911051	-0.675232	-0.567407
H	-0.823151	-2.645363	0.714745
H	-1.819438	-4.921539	0.829521
H	-4.263138	-5.202643	0.294533
H	-5.598588	-3.111719	-0.263601

Table S26. Cartesian coordinates of **5** at the $T_{1,opt}$ optimized geometry.

C	-2.220248	4.521023	-0.057916
C	-0.872994	4.936183	0.087973
C	-2.503872	3.162445	-0.110298
N	-1.540035	2.231938	-0.028633
C	0.121576	3.989256	0.167396
C	-0.196967	2.603136	0.105645
C	0.695015	1.516294	0.133471
C	2.124750	1.646796	0.247303
C	0.068597	0.169862	-0.036472
C	0.912094	-0.899186	-0.278392
C	2.912543	0.555666	0.029215
C	2.313992	-0.745245	-0.249630
Pt	-1.916390	0.256792	0.005118
H	-3.029806	5.238668	-0.125641
H	-0.628173	5.993173	0.131461
H	-3.512263	2.775687	-0.215005
H	1.159235	4.288077	0.268526
H	2.560161	2.614657	0.474059
H	0.505358	-1.883683	-0.487238
C	3.365391	-1.709202	-0.370511
C	4.619467	-1.065482	-0.175528
C	3.316016	-3.098105	-0.615908
C	4.504180	-3.819197	-0.655985
C	5.795384	-1.797563	-0.216950
C	5.738637	-3.180994	-0.455943
C	4.438784	0.443397	0.023309
C	5.079394	0.953922	1.341316
C	4.611009	0.241193	2.614720
C	5.072883	1.160915	-1.215520
C	4.966809	2.688419	-1.284289
H	2.363679	-3.597971	-0.771028
H	4.478969	-4.889385	-0.843706
H	6.758462	-1.314926	-0.067706
H	6.656979	-3.760334	-0.489611
H	6.170337	0.858769	1.247057
H	4.876305	2.027554	1.437152
H	5.111871	0.662056	3.493806
H	3.530973	0.354061	2.759622
H	4.836224	-0.829866	2.580316
H	6.133482	0.876696	-1.238955
H	4.623038	0.730380	-2.118650

H	5.472215	3.051402	-2.186506
H	3.925351	3.020244	-1.338631
H	5.439990	3.178780	-0.426604
C	-1.846592	-2.793760	0.535293
C	-2.414011	-4.059755	0.616775
C	-3.769532	-4.218903	0.321629
C	-3.890027	-1.848631	-0.065972
C	-4.513363	-3.091164	-0.013295
N	-2.558934	-1.709353	0.170189
O	-4.013980	0.515224	-0.176034
C	-4.697307	-0.581445	-0.312249
O	-5.890464	-0.680208	-0.569465
H	-0.806490	-2.621174	0.775310
H	-1.796045	-4.900575	0.914079
H	-4.236425	-5.198243	0.371434
H	-5.576299	-3.121262	-0.224730

Table S28. Cartesian coordinates of **6** at the S_0 optimized geometry.

C	5.885944	-3.461998	0.960280
C	5.620732	-2.120475	0.720662
C	4.823534	-4.369650	0.918532
C	3.538712	-3.912905	0.650626
N	4.373145	-1.687488	0.460865
C	3.313460	-2.547736	0.423737
C	2.034655	-1.890686	0.177749
C	0.806473	-2.579748	0.200731
C	2.105736	-0.475174	-0.004669
C	0.890158	0.218478	-0.058626
C	-0.378434	-1.874143	0.066231
C	-0.329667	-0.465169	-0.024582
C	-1.700786	0.044323	-0.037326
C	-2.589061	-1.047978	0.033983
C	-2.203220	1.347542	-0.091228
C	-3.961201	-0.845568	0.058596
C	-4.472757	0.466510	-0.000813
C	-3.580203	1.553577	-0.080688
C	-1.824739	-2.375430	0.050683
C	-2.174728	-3.249714	1.284662
C	-2.000351	-2.566467	2.645655
C	-2.167348	-3.130893	-1.275655
C	-1.452873	-4.463499	-1.527601
H	6.900890	-3.781116	1.169238
H	6.386014	-1.351525	0.721106
H	4.997095	-5.427549	1.094402
H	2.707009	-4.607158	0.615428
H	0.787597	-3.655999	0.348766
H	0.876033	1.303600	-0.086057
H	-1.533630	2.201833	-0.152483
H	-4.651064	-1.681258	0.127541
N	-5.873873	0.690246	0.016983
H	-3.979213	2.561067	-0.135699
H	-3.213464	-3.592766	1.178077
H	-1.554952	-4.154953	1.258572
H	-2.249144	-3.261163	3.456014
H	-0.968061	-2.232460	2.795181
H	-2.652747	-1.692369	2.741358
H	-3.252404	-3.301394	-1.285171
H	-1.957291	-2.451561	-2.111136
H	-1.790628	-4.890227	-2.479095

H	-0.367721	-4.334363	-1.594438
H	-1.662946	-5.203041	-0.747069
Pt	3.990371	0.240913	-0.021305
N	3.861262	2.210824	-0.653654
C	2.818478	2.829425	-1.239668
C	2.872747	4.161340	-1.634909
C	4.047027	4.885146	-1.423931
C	5.136782	4.233490	-0.854201
C	5.023997	2.894037	-0.494641
C	6.235420	2.122031	0.019433
O	6.029018	0.851109	0.161778
O	7.280113	2.732746	0.211820
H	1.935446	2.226910	-1.399463
H	2.004157	4.612604	-2.102944
H	4.113929	5.929573	-1.714725
H	6.094645	4.712066	-0.684482
C	-6.741515	-0.164974	-0.717724
C	-6.414916	1.775641	0.760776
C	-7.953411	-0.602099	-0.158393
C	-8.805048	-1.431430	-0.886485
C	-8.458834	-1.853431	-2.172290
C	-6.400650	-0.582870	-2.014810
C	-7.250358	-1.426729	-2.728031
C	-5.933133	2.069086	2.047175
C	-6.460557	3.138938	2.768296
C	-7.485626	3.921662	2.231703
C	-7.973343	3.626105	0.956600
C	-7.439833	2.569502	0.220372
H	-8.220848	-0.287586	0.845366
H	-9.739029	-1.759891	-0.437972
H	-9.122095	-2.505138	-2.733792
H	-5.469956	-0.241941	-2.457048
H	-6.970900	-1.739310	-3.730839
H	-5.146133	1.455814	2.474445
H	-6.075741	3.351348	3.762354
H	-7.898945	4.750158	2.799735
H	-8.766258	4.229697	0.522625
H	-7.812933	2.352551	-0.775462

Table S29. Cartesian coordinates of **6** at the $T_{1,opt}$ optimized geometry.

C	5.821697	-3.441509	1.159374
C	5.575488	-2.108450	0.860340
C	4.746956	-4.360664	1.112844
C	3.486696	-3.914637	0.781484
N	4.349682	-1.667534	0.533392
C	3.263920	-2.542487	0.486886
C	2.036677	-1.918239	0.170774
C	0.778724	-2.612244	0.098634
C	2.103583	-0.447167	-0.019026
C	0.911148	0.241127	-0.062876
C	-0.375707	-1.895469	-0.026087
C	-0.334779	-0.442393	-0.052639
C	-1.664437	0.045196	-0.047106
C	-2.581395	-1.053999	-0.045590
C	-2.177901	1.367799	-0.024931
C	-3.939931	-0.846107	-0.014805
C	-4.451006	0.481012	0.014879
C	-3.543834	1.572077	0.003814
C	-1.824222	-2.385075	-0.102445
C	-2.199522	-3.336360	1.064718
C	-2.034930	-2.746921	2.469800
C	-2.139776	-3.053110	-1.482595
C	-1.425539	-4.370372	-1.804854
H	6.826440	-3.755830	1.417810
H	6.351767	-1.350345	0.866332
H	4.913739	-5.409590	1.339816
H	2.651109	-4.605298	0.747596
H	0.755420	-3.694403	0.182129
H	0.901362	1.326746	-0.086762
H	-1.504836	2.220379	-0.037769
H	-4.633914	-1.680655	0.003762
N	-5.839384	0.710286	0.052038
H	-3.939381	2.582332	0.007511
H	-3.240584	-3.658781	0.921072
H	-1.588374	-4.243668	0.985110
H	-2.315189	-3.486090	3.228810
H	-0.997560	-2.450349	2.657953
H	-2.668097	-1.864624	2.611017
H	-3.225515	-3.215002	-1.523200
H	-1.910171	-2.322292	-2.268131
H	-1.740420	-4.729031	-2.791586

H	-0.338844	-4.243787	-1.833785
H	-1.660365	-5.159298	-1.082055
Pt	3.981083	0.233012	-0.013431
N	3.866601	2.186852	-0.695362
C	2.841144	2.787763	-1.331313
C	2.903564	4.109874	-1.754704
C	4.069033	4.844156	-1.525333
C	5.141799	4.209959	-0.905579
C	5.021980	2.879685	-0.515907
C	6.215667	2.124658	0.055698
O	6.007641	0.855620	0.221221
O	7.253853	2.740614	0.269299
H	1.966718	2.175870	-1.505514
H	2.048936	4.546393	-2.261200
H	4.142450	5.880934	-1.840784
H	6.092648	4.695874	-0.717878
C	-6.732196	-0.154630	-0.643527
C	-6.370524	1.809049	0.786701
C	-7.917906	-0.590883	-0.030687
C	-8.792746	-1.429637	-0.718344
C	-8.495553	-1.855048	-2.015724
C	-6.438488	-0.576083	-1.950696
C	-7.313675	-1.425717	-2.624770
C	-5.887064	2.105023	2.071725
C	-6.407457	3.184388	2.783161
C	-7.421976	3.973010	2.234582
C	-7.909741	3.674243	0.959790
C	-7.386801	2.605500	0.234456
H	-8.143704	-0.271762	0.981686
H	-9.705793	-1.761493	-0.231521
H	-9.177844	-2.512701	-2.546434
H	-5.528740	-0.229827	-2.430586
H	-7.075871	-1.741488	-3.636980
H	-5.109460	1.484436	2.505307
H	-6.025899	3.400426	3.777378
H	-7.828485	4.810181	2.794538
H	-8.694395	4.283593	0.519554
H	-7.757723	2.383184	-0.760932

Table S30. Cartesian coordinates of **7** at the S_0 optimized geometry.

C	-2.400983	4.350837	-0.083169
C	-1.144644	4.937730	0.090335
C	-2.484972	2.966254	-0.144977
N	-1.386683	2.193987	-0.047847
C	-0.016445	4.131065	0.187797
C	-0.147196	2.738877	0.112400
C	0.926281	1.748759	0.147376
C	2.284994	2.099969	0.205713
C	0.501148	0.386181	0.038694
C	3.232154	1.096230	0.122117
C	1.501431	-0.597206	-0.099941
C	2.847035	-0.249391	-0.052056
C	4.074383	-1.074354	-0.159198
C	5.194905	-0.225663	-0.040341
C	4.255879	-2.440782	-0.344539
C	5.565704	-2.940437	-0.407516
C	6.490547	-0.715485	-0.101167
C	6.671576	-2.093192	-0.287175
C	4.720942	1.187199	0.141684
O	5.407757	2.187113	0.272126
Pt	-1.499113	0.172383	-0.004320
H	-3.302092	4.948011	-0.166783
H	-1.045255	6.017812	0.148054
H	-3.419553	2.429447	-0.267710
H	0.964644	4.572243	0.320758
H	2.610822	3.132583	0.299264
H	1.230430	-1.632684	-0.277276
H	3.409374	-3.115437	-0.442293
H	5.722365	-4.006012	-0.552989
H	7.334997	-0.038472	-0.007097
H	7.674656	-2.507001	-0.339375
N	-1.881999	-1.859103	0.188210
C	-1.044017	-2.833147	0.591438
C	-1.443646	-4.160851	0.693194
C	-2.758257	-4.501228	0.371844
C	-3.634342	-3.487805	-0.005433
C	-3.176875	-2.175447	-0.071236
O	-3.613834	0.147988	-0.223934
C	-4.141304	-1.029528	-0.357204
O	-5.302905	-1.294832	-0.637961
H	-0.040560	-2.524694	0.848439

H	-0.728976	-4.907037	1.024084
H	-3.094441	-5.532178	0.433323
H	-4.678734	-3.660326	-0.239651

Table S31. Cartesian coordinates of **7** at the $T_{1,opt}$ optimized geometry.

C	-2.310814	4.371842	-0.168800
C	-1.042222	4.945740	0.010937
C	-2.423520	2.987707	-0.202678
N	-1.347221	2.192343	-0.071218
C	0.065115	4.124273	0.140941
C	-0.088952	2.724217	0.095786
C	0.951730	1.738237	0.170095
C	2.313738	2.062728	0.305131
C	0.494322	0.321800	0.019413
C	3.243722	1.055946	0.188896
C	1.464489	-0.648904	-0.165333
C	2.835589	-0.329813	-0.090534
C	4.023623	-1.098967	-0.213177
C	5.166306	-0.242588	-0.010408
C	4.231002	-2.474968	-0.484659
C	5.524243	-2.956082	-0.545682
C	6.465122	-0.748331	-0.075862
C	6.643532	-2.101393	-0.342501
C	4.719896	1.138338	0.248464
O	5.402756	2.145175	0.463253
Pt	-1.493124	0.179662	0.001516
H	-3.199491	4.983157	-0.278382
H	-0.926713	6.024852	0.043922
H	-3.369254	2.471197	-0.328168
H	1.053846	4.548726	0.271568
H	2.655160	3.082149	0.464296
H	1.179753	-1.674797	-0.377559
H	3.387181	-3.140703	-0.645687
H	5.697262	-4.008479	-0.754244
H	7.309476	-0.082798	0.079955
H	7.645052	-2.518377	-0.399444
N	-1.910829	-1.838808	0.208580
C	-1.085644	-2.822347	0.616643
C	-1.506560	-4.142563	0.726466
C	-2.827995	-4.463884	0.412004
C	-3.689576	-3.439384	0.030227
C	-3.211696	-2.135227	-0.046689
O	-3.603267	0.195698	-0.222114
C	-4.154044	-0.975392	-0.342282
O	-5.321143	-1.216936	-0.619210
H	-0.076858	-2.525524	0.868046

H	-0.803032	-4.898310	1.059496
H	-3.180473	-5.488749	0.482219
H	-4.737129	-3.598153	-0.199639

References

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