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Supporting Information

Photoinduced charge separation in a Platinum(II) acetylide donor-acceptor triad based on 2-(1-Pyrazole)-Pyridine modified with Naphthalene mono-imide electron acceptor

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1 1 (^{1}A)

General Information

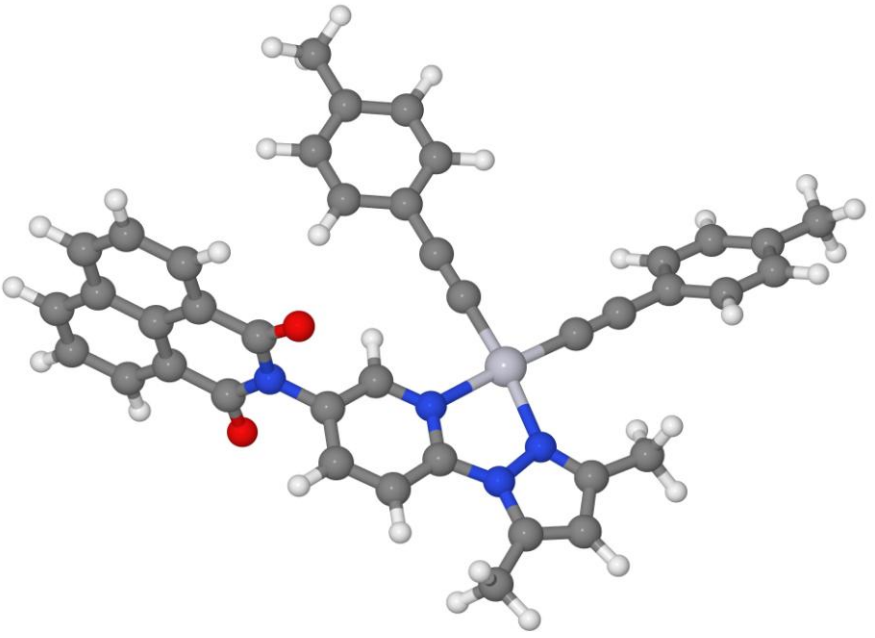

Figure S1: Compound 1: Geometry Singlet S_0 state

Figure S2: Compound 1: Electrostatic Potential Singlet S_0 state

SMILES	:	Cc1ccc(cc1)C#C[Pt]2(n3c(cc([n+]3-c4[n+]2cc(cc4)N5C(=O)c6cccc7c6c(ccc7)C5=O)C)C)C#Cc8ccc(cc8)C
Formula	:	$C_{40}H_{30}N_4O_2Pt$
Charge	:	0
Multiplicity	:	1
Dipole	:	15.9244 Debye
Energy	:	-2031.66719864 a.u.
Number of imaginary frequencies	:	0

1.1 Cartesian Co-ordinates (XYZ format)

77

C	0.98055393	-3.76999784	-0.22387794
C	2.11232901	-4.60245943	-0.35359231
C	3.21731353	-3.79208302	-0.42001209
H	2.11532950	-5.67928457	-0.39127716
C	4.78710318	-1.10925698	-0.45600477
C	5.33241558	0.16384564	-0.44336686
H	5.43335676	-1.96060514	-0.56788361
C	3.13539290	1.05236638	-0.17718917
C	4.49518585	1.26411641	-0.30126762
H	6.40169191	0.29660490	-0.54560024
H	2.43495679	1.86934555	-0.06537785
C	3.40473771	-1.25257707	-0.32770482
N	1.36621773	-2.49670100	-0.20910630
N	2.59870791	-0.17882280	-0.19224964
N	2.74600887	-2.49385691	-0.33087268
Pt	0.50631845	-0.55733073	-0.03756705
C	-0.44333154	-4.19984961	-0.13474378
H	-0.49426273	-5.23268414	0.21186204
H	-1.01226604	-3.55626965	0.53358179
H	-0.91895497	-4.14810610	-1.11860800
C	4.63949203	-4.22313595	-0.55585575
H	5.09652424	-3.85361099	-1.47715700
H	5.25110006	-3.90330338	0.29127538
H	4.66119623	-5.31184816	-0.58870155
C	-2.59015775	-1.26291573	0.14084682
C	-0.34210569	2.49447417	0.21472830
C	-0.72164536	3.86647654	0.32462817
C	-2.07433033	4.25139809	0.24497804
C	0.23469327	4.88228655	0.51115543
C	-2.44465971	5.58670712	0.34823474
H	-2.83045411	3.48926926	0.09688007
C	-0.14776973	6.21514082	0.61357057
H	1.28363645	4.61635780	0.57280391

C	-1.49237239	6.59605742	0.53706533
H	-3.49522877	5.85139227	0.27857533
H	0.61440694	6.97545147	0.75356585
C	-3.97761250	-1.58965707	0.21799034
C	-4.53923464	-2.59266877	-0.59513181
C	-4.83648300	-0.91606009	1.10805535
C	-5.89193249	-2.90430546	-0.51567584
H	-3.90347242	-3.12048650	-1.29658484
C	-6.18660688	-1.23784113	1.18040729
H	-4.43134499	-0.13449255	1.74017668
C	-6.74296188	-2.23846889	0.37409940
H	-6.29555941	-3.67916083	-1.16016662
H	-6.82284403	-0.69797844	1.87497711
C	-0.04019872	1.31464720	0.11813866
C	-1.39667654	-1.01229501	0.07720479
C	-8.20406914	-2.60248995	0.47928435
H	-8.58113766	-3.01227903	-0.46046600
H	-8.36670876	-3.35994220	1.25438917
H	-8.81301498	-1.73420274	0.74198508
C	-1.90566993	8.04075336	0.67939466
H	-2.78895760	8.26364040	0.07607284
H	-2.15466118	8.27850246	1.71976244
H	-1.10378015	8.71649837	0.37363404
C	5.01414633	3.30586982	-1.51511753
C	5.49625349	3.09386516	0.94779992
C	5.54697418	4.68288755	-1.47547257
C	6.02113199	4.47449493	0.93864805
C	6.03317213	5.22812128	-0.26129910
C	5.56848526	5.43560743	-2.63556170
C	6.50093031	5.02588797	2.11282110
C	6.54479647	6.55959797	-0.24686205
C	6.07210732	6.74941444	-2.62455845
H	5.19042587	4.99708223	-3.55032587
C	7.00566816	6.33919668	2.13051796
H	6.48034477	4.43026543	3.01663971
C	6.55041456	7.30043125	-1.45611846
C	7.02774525	7.09072781	0.97618419
H	6.08061171	7.32538939	-3.54166126
H	7.37662315	6.75585604	3.05878186
O	5.46345282	2.38651299	1.93710613
O	4.59255791	2.77000594	-2.52249432
N	5.01297426	2.60425377	-0.28720194
H	6.93856955	8.31279087	-1.44706357
H	7.41639709	8.10293674	0.98926753

1.2 TD-DFT calculations

Table SI-1a: Most important electronic transitions (f>0.04) of **1** in its S_0 state

No.	Energy (cm^{-1})	Wave length (nm)	Osc. Strength	Major contributions
3	21345	468.50	0.06	HOMO → L+! (96%)
4	22892	436.84	0.18	H-1→L+1 (95%)
6	26147	382.45	0.04	H-2→L+1 (88%)
7	26453	378.03	0.05	HOMO→L+2 (83%)
13	29395	340.19	0.34	H-5→LUMO (96%)
20	32333	309.28	0.05	H-11→LUMO (77%), H-5→L+4 (12%)
21	32599	306.76	0.36	HOMO→L+5 (85%)
27	33615	297.49	0.09	H-8→L+1 (82%)
28	34132	292.98	0.04	H-4→L+2 (18%), H-3→L+2 (51%), H-1→ L+5 (14%)
29	34193	292.45	0.07	H-3→L+2 (13%), H-1→L+5 (54%)
31	34533	289.58	0.18	H-1→L+5 (14%), HOMO→L+6 (17%), HOMO→L+11 (36%)
35	35156	284.45	0.45	H-9→L+1 (76%)
36	35580	281.06	0.05	H-2→L+5 (17%), H-1→L+6 (29%), H-1→ L+11 (28%)
37	35706	280.07	0.04	H-2→L+5 (49%), H-2→L+6 (11%), H-1→ L+11 (10%)
39	36543	273.65	0.20	H-10→L+1 (21%), HOMO→L+6 (44%), HOMO→L+11 (19%)
41	37002	270.26	0.14	H-10→L+1 (24%), H-3→L+5 (12%), H-1→ L+6 (20%)
44	37386	267.48	0.08	H-2→L+6 (10%), H-1→L+6 (20%), H-1→ L+11 (11%)
45	37524	266.49	0.16	H-10→L+1 (22%), H-3→L+5 (15%), H-2→ L+6 (13%), HOMO→L+6 (10%)
49	38287	261.19	0.04	HOMO→L+9 (31%)
50	38511	259.67	0.04	H-3→L+5 (15%), H-2→L+11 (20%), HOMO→L+9 (15%)
62	39939	250.38	0.04	H-9→L+2 (16%), HOMO→L+12 (60%)
64	40045	249.72	0.13	H-13→L+1 (11%), H-9→L+2 (29%), H-4→ L+3 (30%)
69	40920	244.38	0.13	H-13→L+1 (64%), H-9→L+2 (15%)
71	41049	243.61	0.05	H-1→L+12 (80%)
76	42062	237.74	0.05	H-3→L+6 (38%), H-2→L+7 (34%)
80	42910	233.05	0.12	H-17→LUMO (39%), H-14→LUMO (11%), H-5→L+3 (16%)
85	43471	230.04	0.05	H-16→L+1 (14%), H-15→L+1 (38%), H-12→L+2 (21%)
86	43578	229.48	0.00	H-4→L+6 (67%)
87	43613	229.29	0.05	H-16→L+1 (62%), H-15→L+1 (15%)
89	43782	228.41	0.47	H-17→LUMO (11%), H-11→LUMO (12%), H-5→L+4 (54%)
91	43934	227.61	0.06	H-3→L+11 (26%)

Table SI-1b: Complete list of electronic transitions of **1** in its S_0 state

No.	Energy (cm^{-1})	Wave length (nm)	Osc. Strength	Major contribs	Minor contribs
1	18719	534.20	0.0001	HOMO->LUMO (93%)	H-1->LUMO (7%)
2	20359	491.18	0.0003	H-1->LUMO (93%)	HOMO->LUMO (7%)
3	21345	468.50	0.0616	HOMO->L+1 (96%)	H-1->L+1 (2%)
4	22892	436.84	0.1825	H-1->L+1 (95%)	HOMO->L+1 (2%)
5	24587	406.72	0.0004	H-2->LUMO (98%)	
6	26147	382.45	0.043	H-2->L+1 (88%)	HOMO->L+2 (8%)
7	26453	378.03	0.0523	HOMO->L+2 (83%)	H-2->L+1 (8%), H-1->L+2 (7%)
8	26880	372.02	0.0001	H-3->LUMO (98%)	
9	27398	364.99	0.0001	H-4->LUMO (94%)	H-4->L+1 (5%)
10	27705	360.94	0.004	H-4->L+1 (75%), H-3->L+1 (18%)	H-4->LUMO (6%)
11	27859	358.96	0.02	H-1->L+2 (90%)	HOMO->L+2 (7%)
12	29108	343.55	0.0192	H-4->L+1 (20%), H-3->L+1 (77%)	
13	29395	340.19	0.3403	H-5->LUMO (96%)	
14	30377	329.20	0.0	H-7->LUMO (100%)	

15	31057	321.99	0.0009	H-12->LUMO (36%), H-9->LUMO (59%)	
16	31265	319.85	0.0135	HOMO->L+3 (91%)	H-1->L+3 (7%)
17	31506	317.40	0.0105	H-2->L+2 (94%)	H-3->L+2 (2%)
18	31716	315.29	0.0	H-8->LUMO (81%), H-6->LUMO (18%)	
19	31728	315.17	0.0	H-8->LUMO (18%), H-6->LUMO (82%)	
20	32333	309.28	0.0484	H-11->LUMO (77%), H-5->L+4 (12%)	H-12->LUMO (7%), H-9->LUMO (2%)
21	32599	306.76	0.357	HOMO->L+5 (85%)	H-1->L+3 (4%), HOMO->L+4 (3%)
22	32682	305.98	0.0063	H-12->LUMO (51%), H-9->LUMO (36%)	H-11->LUMO (8%)
23	32731	305.52	0.0116	HOMO->L+4 (90%)	H-1->L+4 (6%), HOMO->L+5 (3%)
24	32930	303.67	0.0209	H-1->L+3 (85%)	HOMO->L+3 (8%), HOMO->L+5 (3%)
25	33044	302.63	0.0109	H-5->L+1 (98%)	
26	33243	300.81	0.0003	H-4->L+2 (75%), H-3->L+2 (23%)	
27	33615	297.49	0.0873	H-8->L+1 (82%)	H-9->L+1 (5%), H-1->L+5 (4%)
28	34132	292.98	0.0359	H-4->L+2 (18%), H-3->L+2 (51%),	H-9->L+1 (7%), HOMO->L+6 (2%)

				H-1->L+5 (14%)	
29	34193	292.45	0.0693	H-3->L+2 (13%), H-1->L+5 (54%)	H-8->L+1 (2%), H-4->L+2 (4%), HOMO->L+6 (9%), HOMO->L+11 (4%)
30	34345	291.16	0.0006	H-1->L+4 (91%)	HOMO->L+4 (6%)
31	34533	289.58	0.1808	H-1->L+5 (14%), HOMO->L+6 (17%), HOMO->L+11 (36%)	H-8->L+1 (5%), HOMO->L+5 (2%), HOMO->L+7 (5%), HOMO->L+9 (5%), HOMO->L+12 (2%)
32	34606	288.97	0.0021	H-7->L+1 (96%)	
33	34770	287.60	0.0004	H-6->L+1 (95%)	
34	34989	285.80	0.004	H-10->LUMO (96%)	
35	35156	284.45	0.4517	H-9->L+1 (76%)	H-8->L+1 (4%), H-3->L+2 (7%), H-2->L+2 (2%)
36	35580	281.06	0.0547	H-2->L+5 (17%), H-1->L+6 (29%), H-1->L+11 (28%)	H-2->L+6 (6%), H-1->L+7 (3%), H-1->L+9 (2%)
37	35706	280.07	0.0402	H-2->L+5 (49%), H-2->L+6 (11%), H-1->L+11 (10%)	H-2->L+3 (3%), H-1->L+5 (3%), H-1->L+6 (9%)
38	35999	277.78	0.0002	H-16->LUMO (85%)	H-14->LUMO (3%), H-12->L+3 (6%)
39	36543	273.65	0.1978	H-10->L+1 (21%), HOMO->L+6 (44%), HOMO->L+11 (19%)	HOMO->L+7 (4%)
40	36899	271.01	0.0251	HOMO->L+8 (46%), HOMO->L+9 (16%)	H-7->L+1 (3%), H-7->L+5 (7%), H-7->L+6 (4%), H-1->L+7 (3%), H-1->L+8 (8%), H-1->L+9 (4%),

					HOMO->L+7 (6%)
41	37002	270.26	0.1443	H-10->L+1 (24%), H-3->L+5 (12%), H-1->L+6 (20%)	H-2->L+3 (5%), H-2->L+6 (7%), H-1->L+7 (6%), H-1->L+11 (8%), HOMO->L+7 (3%)
42	37061	269.83	0.0134	H-1->L+7 (18%), HOMO->L+7 (29%), HOMO->L+8 (10%)	H-10->L+1 (6%), H-6->L+1 (3%), H-6->L+5 (4%), H-6->L+6 (6%), H-1->L+8 (8%), HOMO->L+9 (4%)
43	37148	269.20	0.0042	H-2->L+3 (81%)	H-3->L+5 (2%), H-2->L+5 (8%), H-2->L+11 (2%)
44	37386	267.48	0.0754	H-2->L+6 (10%), H-1->L+6 (20%), H-1->L+11 (11%)	H-4->L+5 (5%), H-4->L+11 (7%), H-3->L+5 (6%), H-3->L+6 (3%), H-3->L+11 (4%), H-2->L+3 (2%), H-2->L+5 (5%), H-2->L+11 (5%), H-1->L+9 (4%), HOMO->L+11 (3%)
45	37524	266.49	0.1564	H-10->L+1 (22%), H-3->L+5 (15%), H-2->L+6 (13%), HOMO->L+6 (10%)	H-9->L+2 (2%), H-4->L+11 (4%), H-2->L+11 (3%), HOMO->L+9 (3%), HOMO->L+11 (7%)
46	37612	265.88	0.0011	H-5->L+2 (91%)	H-14->LUMO (3%), H-5->L+3 (3%)
47	38053	262.79	0.0048	H-14->LUMO (43%), H-13->LUMO (25%)	H-15->LUMO (6%), H-5->L+2 (6%), H-5->L+3 (9%), H-5->L+4 (7%)
48	38170	261.98	0.0013	H-14->LUMO (16%), H-13->LUMO (71%)	H-5->L+3 (4%), H-5->L+4 (2%)
49	38287	261.19	0.0426	HOMO->L+9	H-10->L+1 (7%), H-9->L+2

				(31%)	(4%), H-8->L+2 (2%), H-4->L+11 (5%), H-1->L+6 (8%), H-1->L+9 (5%), HOMO->L+7 (6%), HOMO->L+8 (7%), HOMO->L+11 (2%)
50	38511	259.67	0.0367	H-3->L+5 (15%), H-2->L+11 (20%), HOMO->L+9 (15%)	H-4->L+6 (2%), H-4->L+11 (7%), H-3->L+11 (2%), H-1->L+6 (5%), H-1->L+11 (4%), HOMO->L+7 (4%), HOMO->L+8 (3%), HOMO->L+11 (4%)
51	38616	258.96	0.0061	H-4->L+11 (12%), H-2->L+4 (30%), H-2->L+11 (16%)	H-4->L+3 (3%), H-4->L+5 (9%), H-4->L+6 (3%), HOMO->L+9 (4%), HOMO->L+11 (2%)
52	38652	258.72	0.0001	H-11->L+1 (92%)	H-14->L+1 (3%), H-2->L+4 (3%)
53	38658	258.68	0.0055	H-2->L+4 (64%), H-2->L+11 (11%)	H-11->L+1 (3%), H-4->L+5 (4%), H-4->L+11 (3%), H-3->L+5 (2%)
54	38957	256.69	0.0028	H-12->L+1 (89%)	H-8->L+2 (3%), H-5->L+3 (2%)
55	39030	256.21	0.0073	H-8->L+2 (88%)	H-12->L+1 (3%)
56	39142	255.48	0.0056	H-17->LUMO (31%), H-5->L+3 (56%)	H-14->LUMO (5%), H-12->L+1 (3%), H-5->L+4 (2%)
57	39407	253.76	0.0036	H-3->L+3 (61%), H-1->L+9 (10%)	H-1->L+7 (5%), H-1->L+8 (2%), H-1->L+11 (5%)
58	39465	253.39	0.0004	H-1->L+7 (38%), H-1->L+8 (11%), HOMO->L+7	H-3->L+3 (2%)

				(29%), HOMO->L+8 (11%)	
59	39500	253.17	0.0044	H-3->L+3 (27%), H-1->L+8 (10%), H-1->L+9 (25%)	H-10->L+1 (3%), H-9->L+2 (3%), H-7->L+2 (6%), H-1->L+7 (3%), H-1->L+11 (8%), HOMO->L+9 (3%)
60	39563	252.76	0.0025	H-7->L+2 (91%)	H-1->L+8 (2%)
61	39900	250.63	0.005	H-1->L+8 (45%), H-1->L+9 (21%), HOMO->L+8 (11%)	H-1->L+7 (8%), HOMO->L+7 (2%), HOMO->L+9 (5%), HOMO->L+12 (2%)
62	39939	250.38	0.0409	H-9->L+2 (16%), HOMO->L+12 (60%)	H-13->L+1 (5%), H-4->L+3 (5%), HOMO->L+11 (2%)
63	39994	250.04	0.0291	H-4->L+3 (54%), HOMO->L+12 (19%)	H-13->L+1 (2%), H-9->L+2 (8%), H-1->L+9 (3%)
64	40045	249.72	0.1274	H-13->L+1 (11%), H-9->L+2 (29%), H-4->L+3 (30%)	H-10->L+1 (2%), H-1->L+9 (7%), HOMO->L+12 (8%)
65	40144	249.10	0.0001	H-6->L+2 (100%)	
66	40160	249.00	0.0	HOMO->L+10 (85%)	H-1->L+10 (7%), HOMO->L+11 (5%)
67	40347	247.85	0.0029	H-3->L+5 (21%), H-2->L+6 (40%)	H-13->L+1 (3%), H-9->L+2 (4%), H-3->L+6 (6%), H-2->L+5 (9%), H-2->L+11 (8%)
68	40654	245.98	0.0163	H-4->L+5 (69%)	H-4->L+6 (4%), H-4->L+11 (7%), H-3->L+5 (6%), H-1->L+12 (3%)
69	40920	244.38	0.1331	H-13->L+1 (64%), H-9->L+2 (15%)	H-14->L+1 (3%), H-1->L+12 (7%)

70	40955	244.17	0.0011	H-3->L+4 (97%)	
71	41049	243.61	0.0477	H-1->L+12 (80%)	H-13->L+1 (6%), H-9->L+2 (2%), H-4->L+5 (2%), H-1->L+11 (3%)
72	41310	242.07	0.0008	H-15->LUMO (87%), H-14->LUMO (10%)	
73	41453	241.24	0.0179	H-15->L+1 (10%), H-14->L+1 (75%)	H-17->LUMO (2%), H-11->L+1 (3%)
74	41542	240.72	0.0001	H-4->L+4 (99%)	
75	41809	239.18	0.0001	H-1->L+10 (88%)	H-1->L+11 (4%), HOMO->L+10 (7%)
76	42062	237.74	0.0464	H-3->L+6 (38%), H-2->L+7 (34%)	H-4->L+6 (2%), H-3->L+5 (4%), H-3->L+11 (4%), H-2->L+8 (2%)
77	42136	237.33	0.0208	H-3->L+6 (18%), H-2->L+7 (32%), H-2->L+8 (23%), H-2->L+9 (11%)	H-3->L+11 (2%), H-2->L+11 (3%)
78	42615	234.66	0.017	H-10->L+2 (83%)	H-2->L+9 (3%)
79	42789	233.71	0.0246	H-2->L+7 (12%), H-2->L+8 (14%), H-2->L+9 (40%)	H-10->L+2 (9%), H-3->L+6 (5%), H-3->L+11 (3%), H-2->L+11 (8%)
80	42910	233.05	0.1231	H-17->LUMO (39%), H-14->LUMO (11%), H-5->L+3 (16%)	H-15->LUMO (2%), H-14->L+1 (3%), H-12->L+2 (2%), H-11->L+2 (7%), H-5->L+4 (7%)
81	43036	232.37	0.0006	H-7->L+3 (99%)	
82	43225	231.35	0.0013	H-12->L+2 (38%), H-11->L+2 (46%)	H-14->L+2 (2%), H-9->L+3 (2%)
83	43265	231.13	0.0003	H-3->L+8 (17%),	H-4->L+8 (2%), H-3->L+7

				H-2->L+8 (36%), H-2->L+9 (25%)	(3%), H-3->L+9 (7%), H-2->L+7 (6%)
84	43300	230.95	0.0017	H-15->L+1 (14%), H-12->L+2 (25%), H-11->L+2 (31%)	H-17->LUMO (6%), H-16->L+1 (6%), H-9->L+3 (3%), H-5->L+3 (2%)
85	43471	230.04	0.0492	H-16->L+1 (14%), H-15->L+1 (38%), H-12->L+2 (21%)	H-14->L+1 (4%), H-11->L+2 (5%)
86	43578	229.48	0.003	H-4->L+6 (67%)	H-16->L+1 (4%), H-4->L+11 (7%), H-3->L+6 (6%), H-3->L+11 (5%), HOMO->L+13 (2%)
87	43613	229.29	0.0466	H-16->L+1 (62%), H-15->L+1 (15%)	H-9->L+3 (2%), H-3->L+6 (3%), H-3->L+11 (3%)
88	43692	228.87	0.0193	H-12->L+3 (12%), H-9->L+3 (66%)	H-16->LUMO (2%), H-16->L+1 (6%), H-12->L+2 (6%), H-5->L+4 (2%)
89	43782	228.41	0.4747	H-17->LUMO (11%), H-11->LUMO (12%), H-5->L+4 (54%)	H-18->LUMO (3%), H-16->L+1 (2%), H-14->LUMO (3%), H-11->L+2 (3%), H-11->L+10 (6%), H-5->L+3 (2%)
90	43905	227.76	0.026	H-18->LUMO (91%)	H-5->L+4 (2%)
91	43934	227.61	0.0631	H-3->L+11 (26%)	H-18->LUMO (3%), H-15->L+1 (5%), H-4->L+6 (6%), H-4->L+9 (3%), H-4->L+11 (7%), H-3->L+6 (5%), H-3->L+7 (4%), H-3->L+9 (6%), H-1->L+13 (9%), HOMO->L+13 (4%)
92	44011	227.22	0.0189	HOMO->L+13	H-15->L+1 (4%), H-3-

				(82%)	>L+11 (2%)
93	44247	226.00	0.0002	H-7->L+4 (100%)	
94	44270	225.89	0.0014	H-8->L+3 (96%)	
95	44406	225.19	0.0006	H-6->L+3 (99%)	
96	44415	225.15	0.0005	H-4->L+7 (11%), H-4->L+8 (11%), H-4->L+9 (43%), H-4->L+11 (10%), H-3->L+9 (12%)	H-3->L+7 (3%), H-3->L+8 (3%)
97	44589	224.27	0.0024	H-11->L+3 (88%)	H-17->L+4 (6%)
98	45003	222.21	0.0093	H-2->L+12 (88%)	H-2->L+11 (4%)
99	45128	221.59	0.0055	H-1->L+13 (76%)	H-13->L+2 (2%), H-3->L+11 (4%)
100	45237	221.06	0.001	H-12->L+3 (66%), H-9->L+3 (19%)	H-16->LUMO (4%)

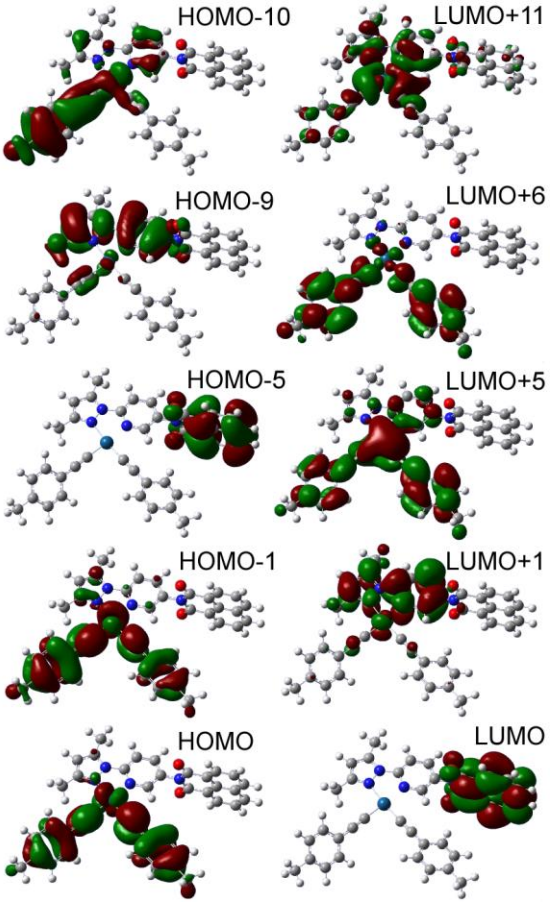

Figure S3a: Compound 1: Selected orbitals for Singlet S_0 state (relate to Table SI-1a)

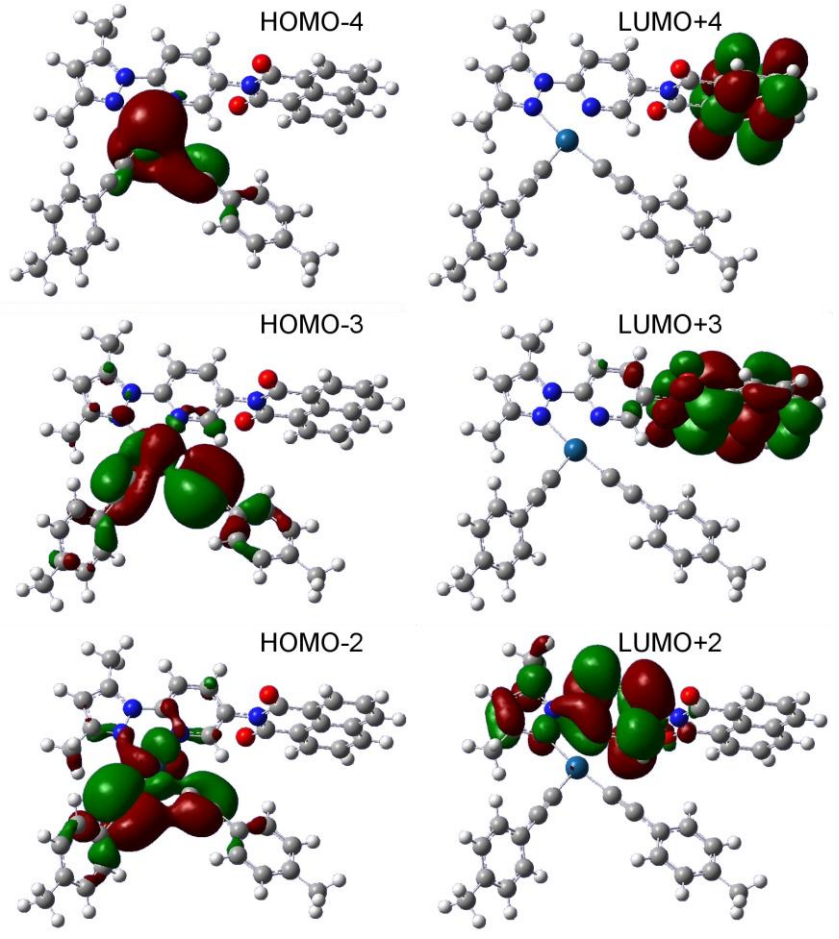

Figure S3a: Compound 1: Orbitals for Singlet S_0 state which participate in less intense transitions (relate to Table SI-1a and 1b)

2 1 Lowest triplet state

2.1 General Information

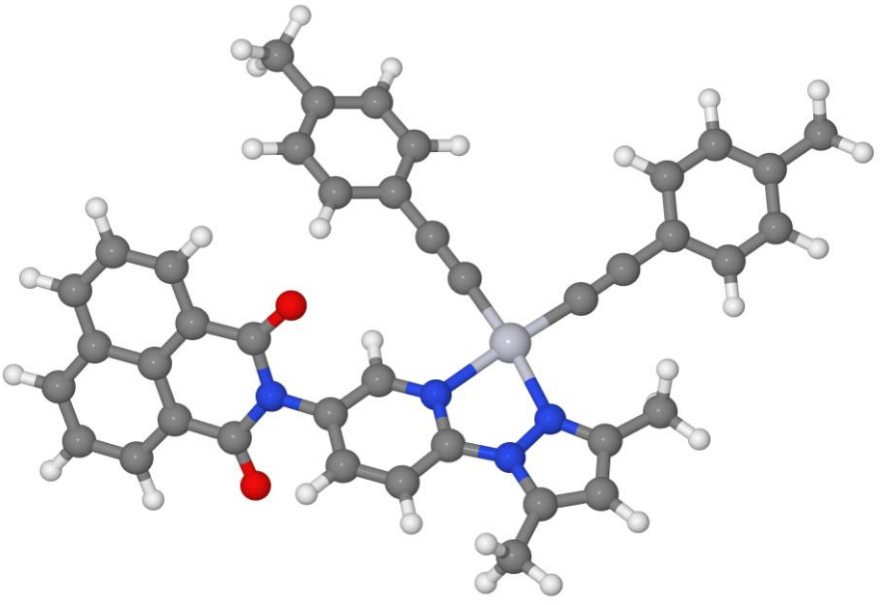

Figure S4: Compound 1: Triplet charge-separated (lowest) state

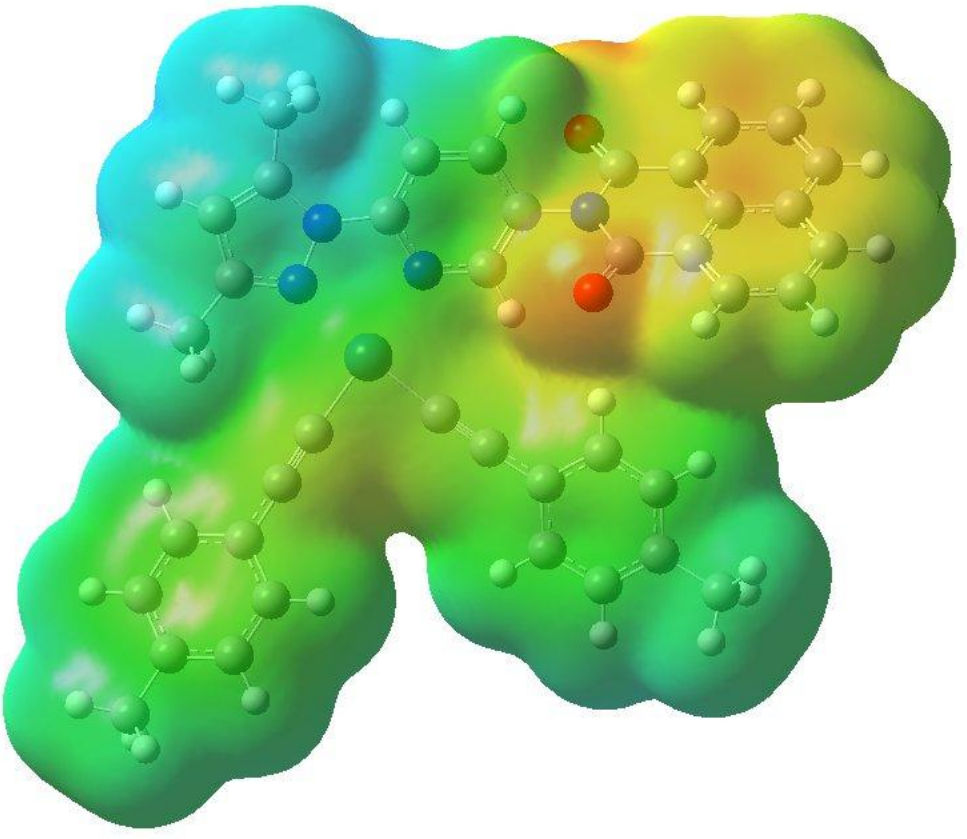

Figure S5: Compound 1: Electrostatic Potential for triplet charge-separated state

SMILES	:	Cc1ccc(cc1)C#C[Pt]2(n3c(cc([n+]3-c4[n+]2cc(cc4)N5C(=O)c6cccc7c6c(ccc7)C5=O)C)C)C#Cc8ccc(cc8)C	
Formula	:	$C_{40}H_{30}N_4O_2Pt^3$	
Charge	:	0	
Multiplicity	:	3	
Dipole	:	15.9244	Debye
Energy	:	-2031.58508924	a.u.
Number of imaginary frequencies	:	0	

Cartesian Co-ordinates (XYZ format)

77

C	-3.36841273	-3.60872459	0.05228333
C	-2.99206138	-4.95093632	-0.11772806
C	-1.61805129	-4.98983383	-0.20790039
H	-3.65195560	-5.80098152	-0.16942969
C	1.28278136	-3.84755707	-0.12286832
C	2.49534655	-3.17676377	-0.05603545
H	1.27733397	-4.91725016	-0.22873828
C	1.30084753	-1.13167000	0.16902694
C	2.51816964	-1.79306388	0.10449906
H	3.41823959	-3.73409462	-0.11634423
H	1.25011313	-0.06289683	0.29038474
C	0.10189352	-3.11556053	-0.05484696
N	-2.27284670	-2.84352040	0.06588341
N	0.12362424	-1.77298224	0.07061215
N	-1.18733561	-3.68733788	-0.09225432
Pt	-1.77152562	-0.79243904	0.08821204
C	-4.74845839	-3.06722212	0.19842060
H	-5.46018648	-3.89103770	0.24719498
H	-4.83839464	-2.46404552	1.10290027
H	-5.00769091	-2.42498922	-0.64532244
C	-0.76642847	-6.19956875	-0.39661890
H	-0.14595979	-6.13002443	-1.29295576
H	-0.11824486	-6.38340139	0.46392983
H	-1.42217839	-7.06199789	-0.50867587
C	-4.65285778	0.55755740	0.06798779
C	-0.54984623	2.10083961	-0.09767727
C	0.09397817	3.32677388	-0.25840595
C	-0.59142733	4.55071545	-0.02643932
C	1.45599449	3.37049198	-0.66952962
C	0.06185623	5.75296307	-0.18979633
H	-1.62908196	4.52169609	0.28120583
C	2.08853173	4.58554792	-0.83073521
H	1.97844434	2.44108725	-0.87235671
C	1.41295624	5.79814959	-0.59160858
H	-0.46874583	6.68099928	-0.00993877
H	3.12492895	4.60863113	-1.14797544
C	-5.92830133	1.18570983	0.05139398
C	-7.09397507	0.48583448	0.42290828
C	-6.06435823	2.53242636	-0.34355146
C	-8.33375168	1.10937440	0.39995843
H	-7.01457357	-0.55053973	0.72824329
C	-7.31005907	3.14336133	-0.36453924
H	-5.18137264	3.08693099	-0.63808292
C	-8.46877289	2.44836092	0.00866196
H	-9.21605968	0.54753393	0.68860179
H	-7.38801765	4.17935562	-0.67781109
C	-1.07572317	0.98514497	0.01831407
C	-3.56297135	0.00355615	0.08031487
C	-9.81403351	3.12848163	0.01415927
H	-10.62339878	2.41246414	-0.14306237
H	-9.99617386	3.62209153	0.97543490
H	-9.87577057	3.89518666	-0.76126999
C	2.12189913	7.11226320	-0.73715693

H	1.43661010	7.90442419	-1.04453290
H	2.55514169	7.41168404	0.22477253
H	2.93956041	7.04816055	-1.45682180
C	3.91641474	0.04910828	-0.66878557
C	4.68339634	-1.52250159	1.16911697
C	5.18217230	0.72891182	-0.57798028
C	5.92703629	-0.79149902	1.23170900
C	6.16146803	0.30681095	0.36286560
C	5.44871044	1.82409370	-1.43695617
C	6.91373920	-1.18391776	2.16652060
C	7.41536808	1.01180077	0.44133461
C	6.66225576	2.49262881	-1.35776377
H	4.69286251	2.11480570	-2.15486121
C	8.11811447	-0.49859023	2.23618340
H	6.70454979	-2.02409387	2.81560755
C	7.63531637	2.10395765	-0.43611211
C	8.37477016	0.58184391	1.39121401
H	6.85886765	3.32773638	-2.02236843
H	8.87038612	-0.80601895	2.95522785
O	4.39558172	-2.48853636	1.88808107
O	2.99516630	0.37167099	-1.43955708
N	3.73918509	-1.06797290	0.20058675
H	8.57965755	2.63549280	-0.38166216
H	9.32070732	1.10994589	1.45288599

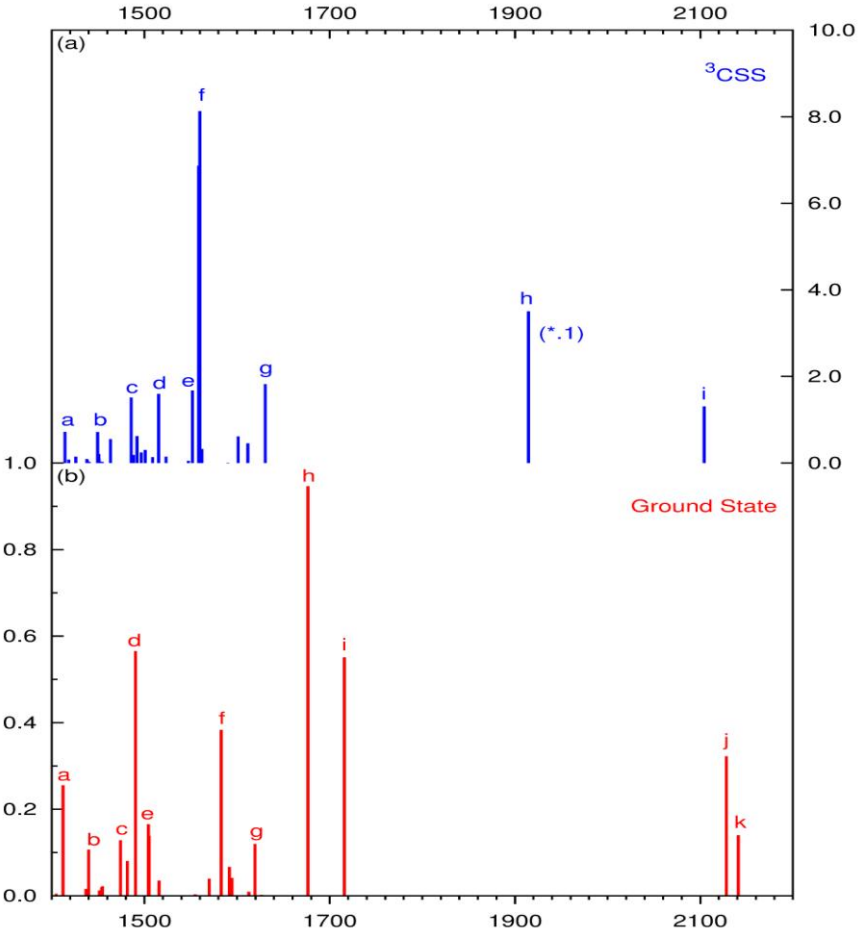

Figure S6**.** Calculated vibrational spectra for **1**.

a: ^{3}Charge-separated state (^{3}CSS) state with the following peak assignments; a - CH_3 scissor mode; b - CH_3 scissor mode; c - Pzpy wagging + CH_3 scissor modes; d - CH wagging of NAP unit; e - CH wagging of NAP unit + asymmetric n(C=O); f - CH wagging in the entire complex; g – symmetric ν(C=O); h – asymmetric n(CC) acetylide; i – symmetric ν(CC) acetylide.

b: Singlet ground state with the following peak assignments; a – CH_3 scissor mode; b – CH wagging NAP + CH_3 scissor mode; c – CH wagging Pzpy group; d – CH wagging Pzpy; e – CH wagging of the Phenyl group; f – CH wagging of the NAP; g – CH wagging of Py; h – asymmetric ν(CO); i – symmetric ν(CO); j – asymmetric ν(CC); k – symmetric ν(CC).

2.2 TD-DFT calculations

Table S-II: Most important transitions (f>0.04) from 1 (^{3}CSS, T_1)

No.	Energy (cm^{-1})	Wave length (nm)	Osc. Strength	Major contribs
16	14879	672.11	0.29	H-11(B)->LUMO(B) (51%), H-9(B)->LUMO(B) (29%)
20	16162	618.74	0.05	H-14(B)->LUMO(B) (75%)
34	25229	396.37	0.13	H-2(A)->LUMO(A) (10%), H-1(A)->LUMO(A) (68%)
35	25363	394.27	0.20	H-2(A)->LUMO(A) (37%), H-1(A)->LUMO(A) (23%), H-1(B)->L+1(B) (26%)
36	25828	387.17	0.29	HOMO(A)->L+12(A) (47%), HOMO(B)->L+2(B) (32%)
38	26257	380.85	0.05	H-21(B)->LUMO(B) (13%), H-19(B)->LUMO(B) (43%), H-18(B)->LUMO(B) (17%)
40	27186	367.84	0.05	H-18(B)->LUMO(B) (69%)
41	27768	360.12	0.07	HOMO(B)->L+3(B) (53%)
42	27791	359.83	0.16	H-4(A)->LUMO(A) (14%), H-3(A)->LUMO(A) (15%), H-19(B)->LUMO(B) (13%), HOMO(B)->L+3(B) (22%)
50	29629	337.51	0.06	H-4(A)->LUMO(A) (22%), H-3(A)->LUMO(A) (14%), H-3(B)->L+1(B) (30%)
65	31512	317.34	0.07	H-5(A)->LUMO(A) (45%), H-5(B)->L+1(B) (22%)
73	32470	307.98	0.06	H-7(A)->LUMO(A) (25%), H-2(A)->L+2(A) (16%), H-5(B)->L+1(B) (13%)
74	32778	305.08	0.17	H-7(A)->LUMO(A) (11%), H-2(A)->L+2(A) (46%)
77	33421	299.22	0.09	H-3(A)->L+1(A) (12%), H-10(B)->L+1(B) (12%), H-1(B)->L+4(B) (21%)
78	33617	297.47	0.04	H-9(A)->LUMO(A) (23%), H-2(A)->L+2(A) (13%), H-7(B)->L+1(B) (24%)
89	34786	287.47	0.04	H-3(A)->L+1(A) (13%)
95	35216	283.96	0.05	H-4(A)->L+1(A) (10%)
96	35291	283.36	0.08	H-8(A)->L+7(A) (21%), H-6(B)->L+9(B) (17%)
97	35412	282.39	0.06	HOMO(A)->L+20(A) (10%), H-5(B)->L+2(B) (18%), H-3(B)->L+3(B) (15%)

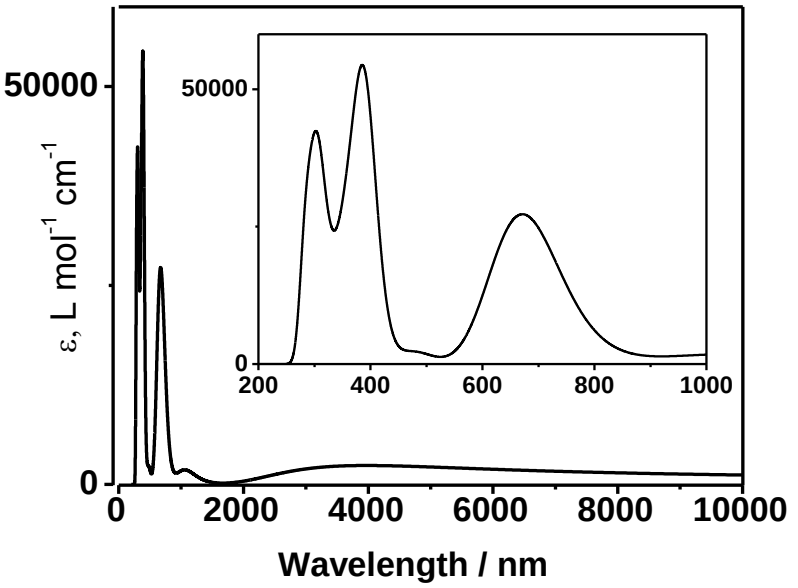

Fig. S7. Calculated UV-Vis spectrum of the triplet charge-separated state. Note that electronic absorption extends into the IR range.