Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Structural, Spectroscopic and Theoretical Studies of A Vapochromic Platinum(II) Terpyridyl Complex

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Figure S1. Solution of **1** (1.65×10^{-5} M) in acetonitrile with increasing diethyl ether content. From left to right: 65%, 68%, 72%, 78%, 80%, 84%, 86%, 88% (v/v).

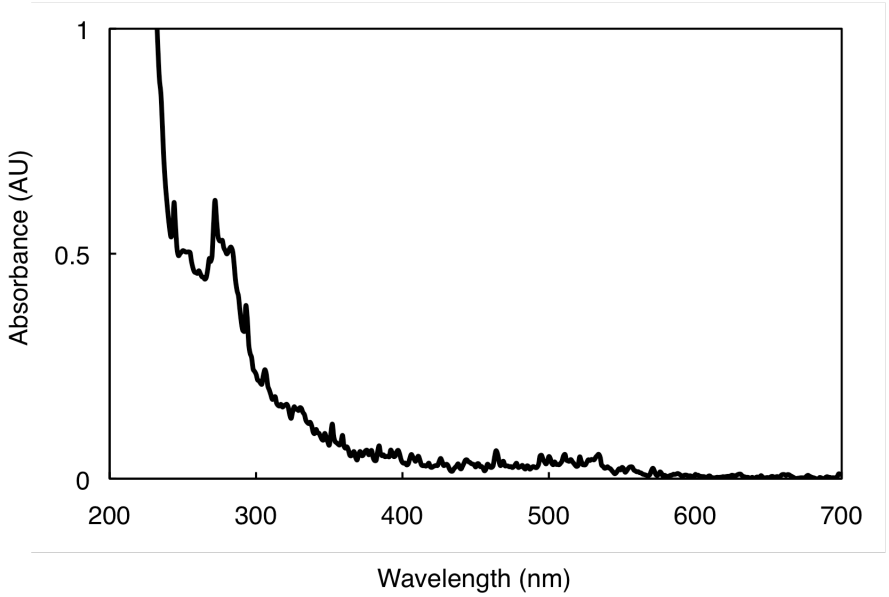

Figure S2. UV-vis spectrum of **1** (1.65×10^{-5} M) in acetonitrile with 90% diethyl ether content.

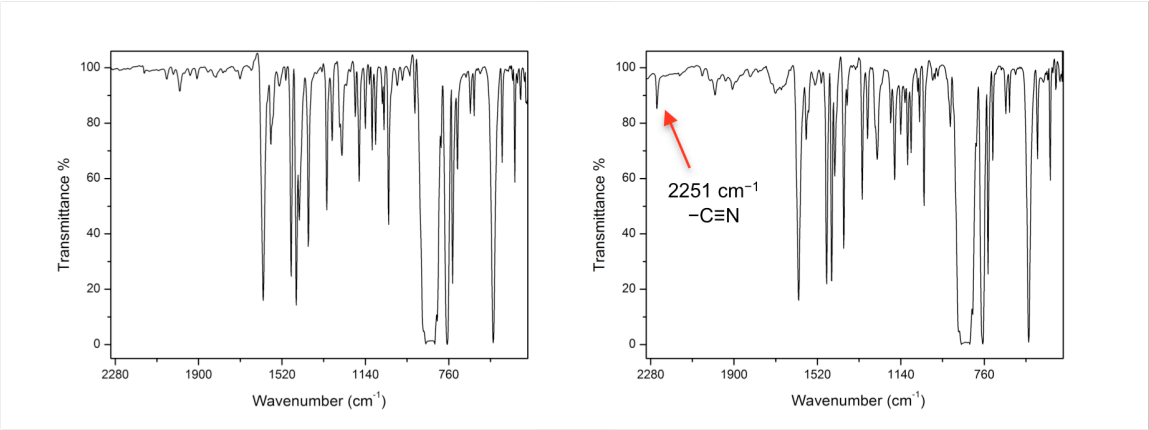

Figure S3. FTIR spectra of **1** (left) and **1**-MeCN (right). The −C≡N bond stretch at 2251 cm^{-1} in **1**-MeCN is successfully located in FTIR.

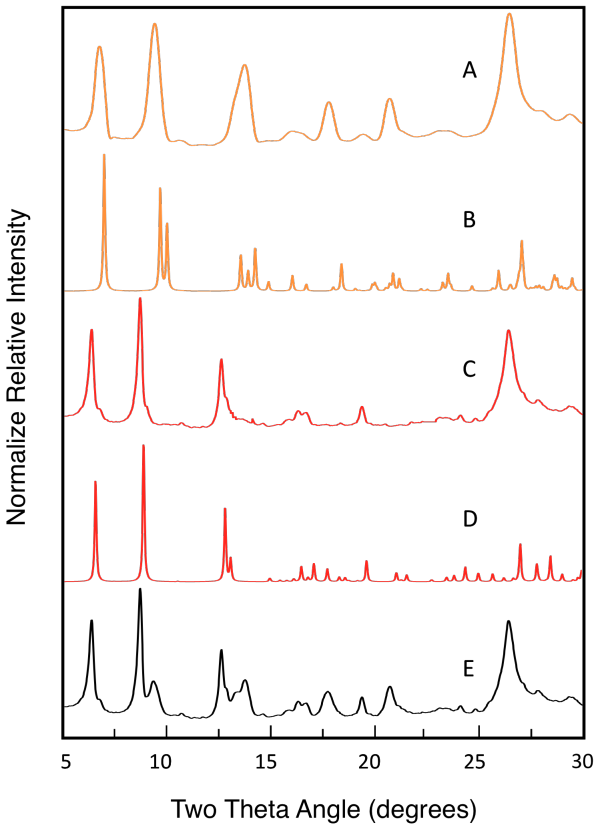

Figure S4. Powder X-ray diffraction data. A) Experimental data of **1**; B) Calculated diffraction pattern of **1**; C) Experimental data of **1**-MeCN; D) Calculated diffraction pattern of **1**-MeCN; E) Powder X-ray diffraction data of a mixture of **1** and **1**-MeCN.

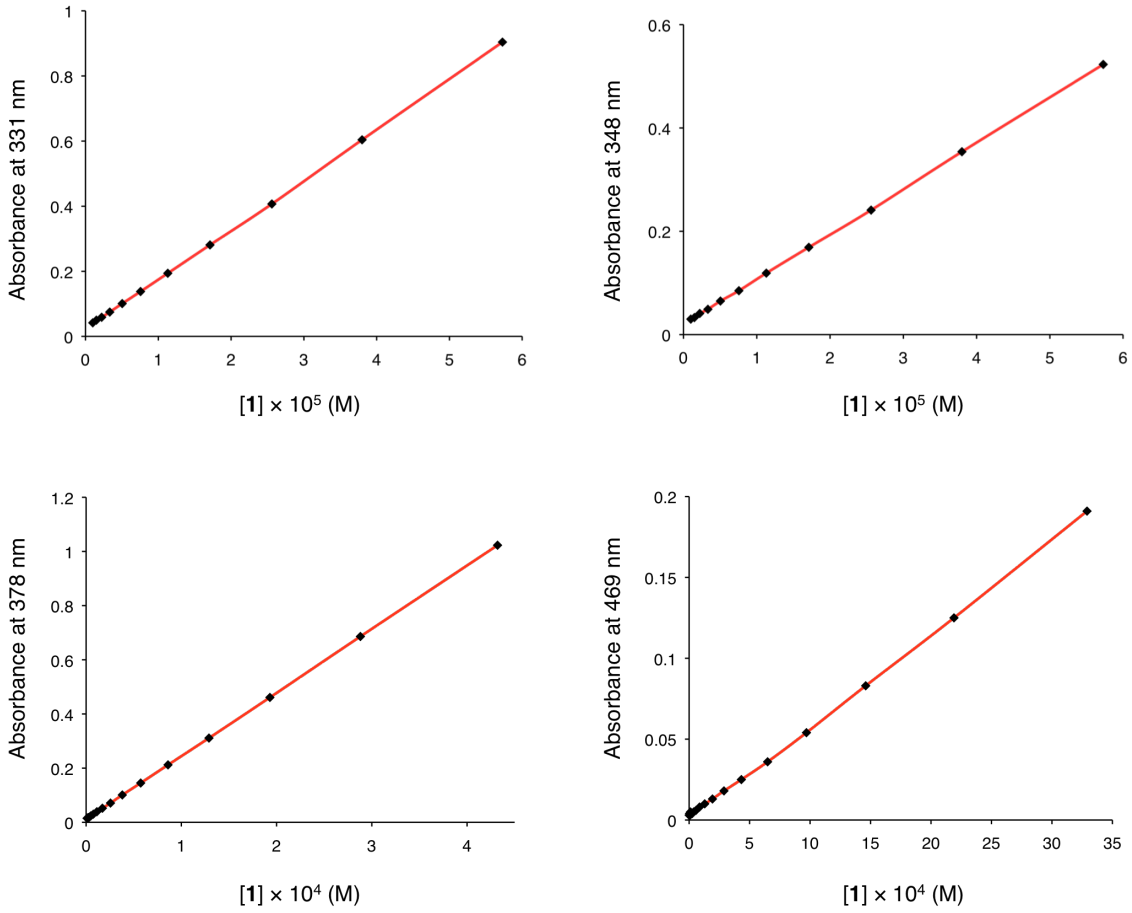

Figure S5. UV-vis absorbance of **1** at 331, 348, 378, 469 nm with different concentration of **1** in acetonitrile.

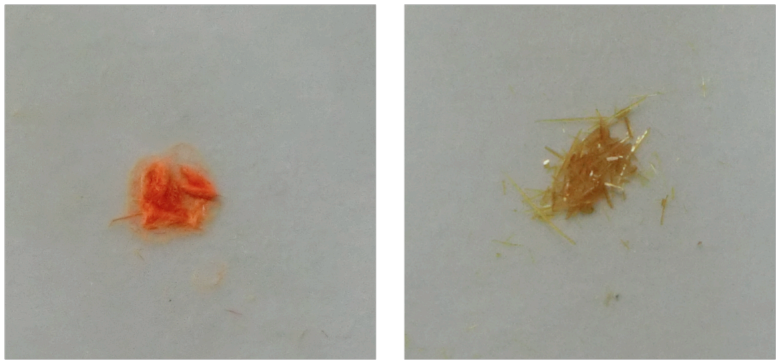

Figure S6. The red and yellow crystals of complex [Pt(tpy)Cl](SbF_6) obtained from acetonitrile (left) and DMF (right).

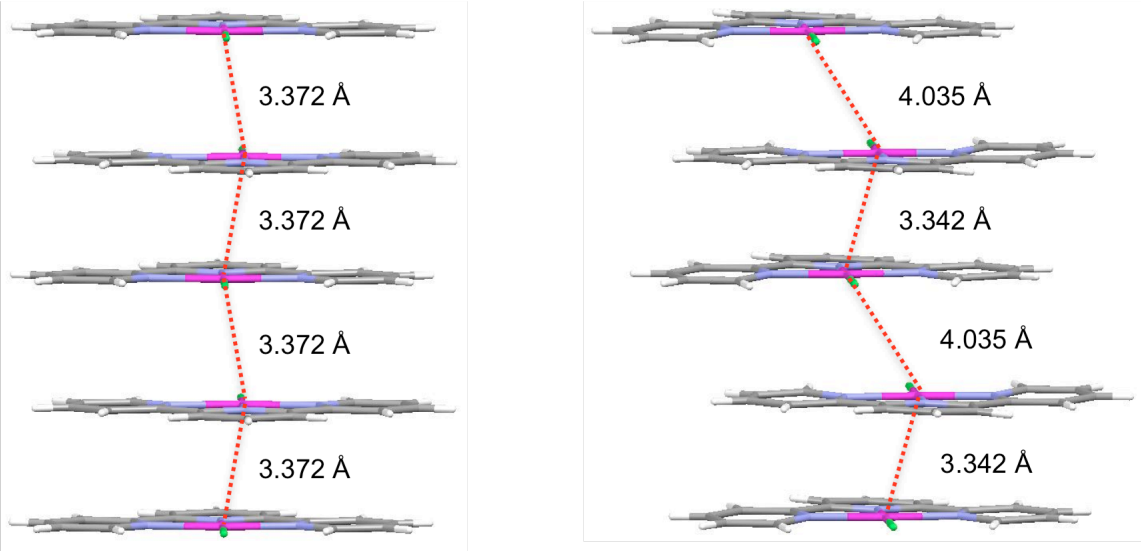

Figure S7. The packing diagram of $[Pt(tpy)Cl]^+$ plane in the red (left) and yellow (right) crystals of $[Pt(tpy)Cl](SbF_6)$.

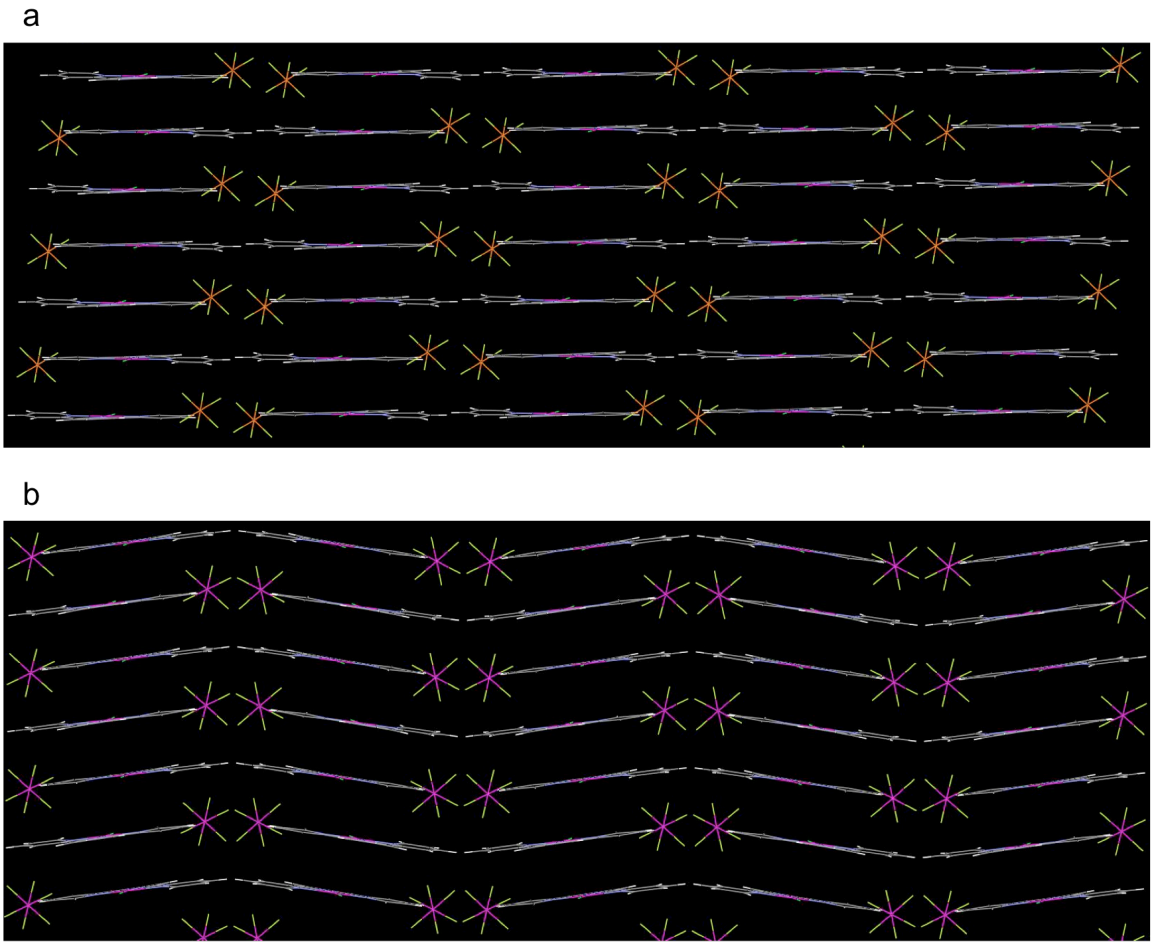

Figure S8. The packing diagrams of $[Pt(tpy)Cl]^+$ and PF_6^- in the X-ray structure of **1** (a) and of $[Pt(tpy)Cl]^+$ and SbF_6^- in the X-ray structure of **2** (b).

Table S1. Crystal data and structure refinement parameters for the X-ray structure of **1**-MeCN

complex	**1**-MeCN
molecular formula	$C_{17}H_{14}ClF_6N_4PPt$
formula wt. (g mol^{-1})	649.83
temperature (K)	153(2)
radiation (λ, Å)	0.71073
crystal system	Orthorhombic
space group	*Pnma* (#62)
a (Å)	27.144(5)
b (Å)	6.5905(13)
c (Å)	10.766(2)
α (°)	
β (°)	
γ (°)	
Volume (Å^3)	1926.0(7)
Z	4
ρ_{calcd} (g cm^{-3})	2.241
μ (mm^{-1})	7.576
F(000)	1232
crystal size (mm^3)	0.46 × 0.08 × 0.07
Theta range	2.94 to 31.50°
reflections collected	18608
indep. reflections	3432 [R(int) = 0.0531]
Completeness	99.6%
Data/restraints/parameters	3432/0/176
goodness-of-fit on F^2	1.064
final R indices	R_1[a] = 0.0434
[R > 2σ (I)]	wR_2[b] = 0.0978
R indices (all data)	R_1[a] = 0.0502
	wR_2[b] = 0.1025
largest diff. peak and hole (e Å^{-3})	2.715 and -2.205

[a] $R_1 = \Sigma||F_o| - |F_c|| / |F_o|$, [b] $wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma[w(F_o^2)^2]\}^{0.5}$

Table S2. The Pt···Pt distances in the 1D line and between 2D arrays of the X-ray structures of the non-solvated yellow form of **1** and **2**

Crystal	**1**	**2**
Pt···Pt distance in the 1D line (Å)	10.027	9.955
Pt···Pt distance between 2D arrays (Å)	4.032 and 3.340	4.035 and 3.342

Table S3. Calculated singlet excited-states transitions for the dimeric form of **1** with Pt···Pt distance of 3.362 Å in acetonitrile

No	nm	*f*	Assignment; H=HOMO, L=LUMO
1	515.1	0.0259	H→L(+97%)
2	493.5	0.0000	H→L+1(+97%)
3	427.8	0.0000	H-1→L(+57%); H→L+2(41%)
4	424.5	0.0000	H→L+2(+57%); H-1→L(+40%)
5	420.8	0.0003	H→L+3(+97%)
6	411.0	0.0507	H-2→L(+79%); H-1→L+1(+15%)
7	408.0	0.0040	H-1→L+1(+81%); H-2→L(18%)
8	393.4	0.0000	H-2→L+1(+65%); H-3→L(14%); H-5→L(+12%)
9	391.3	0.0000	H-3→L(+71%); H-2→L+1(+18%); H-4→L+1(+5%)
10	389.7	0.0002	H-4→L(+82%); H-3→L+1(+10%); H-5→L+1(+6%)
11	388.8	0.0000	H-5→L(+68%); H-2→L+1(12%); H-4→L+1(+11%); H-6→L+1(+5%)
12	383.1	0.0028	H-6→L(+40%); H-5→L+1(+31%); H-3→L+1(25%)
13	376.2	0.0236	H-1→L+2(+89%); H-2→L+3(+7%)
14	373.6	0.0000	H-1→L+3(+77%); H-2→L+2(+19%)
15	367.1	0.0032	H-3→L+1(+51%); H-5→L+1(+30%); H-4→L(17%)
16	366.5	0.0000	H-4→L+1(+81%); H-5→L(9%); H-3→L(8%)
17	357.7	0.0000	H-2→L+2(+79%); H-1→L+3(19%)
18	354.6	0.0055	H-2→L+3(+90%); H-1→L+2(8%)
19	348.4	0.0083	H-6→L(+56%); H-5→L+1(30%); H-3→L+1(+11%)
20	342.3	0.0000	H-6→L+1(+82%); H-5→L(9%)
21	335.5	0.0024	H-3→L+2(+63%); H-5→L+2(+20%); H-4→L+3(+15%)
22	335.0	0.0000	H-4→L+2(+74%); H-3→L+3(+18%)
23	332.3	0.0000	H-7→L(+42%); H-9→L(+40%)
24	329.6	0.0000	H-3→L+3(+50%); H-5→L+3(+26%); H-4→L+2(21%)
25	329.2	0.0114	H-4→L+3(+81%); H-3→L+2(13%)
26	327.8	0.0494	H→L+9(+50%); H-5→L+2(29%)
27	326.2	0.0000	H→L+8(+63%); H-7→L(10%)
28	324.7	0.0058	H→L+4(+95%)
29	322.8	0.0000	H-8→L+1(+47%) H-7→L(+37%); H-9→L+1(6%)
30	322.2	0.0321	H-8→L+1(+46%); H-7→L+1(+20%); H-5→L+2(12%); H→L+9(+8%); H-3→L+2(5%)
31	321.4	0.0252	H-5→L+2(+52%); H→L+9(+24%); H-8→L+1(16%); H-7→L+1(11%); H-3→L+2(11%)
32	320.6	0.0000	H→L+5(+74%); H→L+7(10%)
33	316.9	0.0000	H-5→L+3(+46%); H-3→L+3(19%); H→L+8(+11%); H→L+5(+9%)
34	314.9	0.0097	H→L+6(+94%)
35	312.6	0.0000	H→L+7(+85%); H→L+5(+12%)
36	311.7	0.3805	H-9→L(+77%)
37	308.0	0.0000	H-6→L+2(+829%); H-9→L+2(+6%)
38	307.2	0.0625	H-7→L+1(+53%); H-8→L+1(+27%); H-9→L(+12%)
39	304.3	0.0205	H-6→L+3(+79%); H-9→L+3(+5%)
40	304.2	0.0000	H-9→L+1(+85%); H-7→L(+7%)
41	297.7	0.0000	H-1→L+9(+56%); H-2→L+8(+39%)
42	297.6	0.0000	H-1→L+8(+56%); H-2→L+9(+38%)
43	294.0	0.0000	H-1→L+4(+86%)
44	292.5	0.0111	H-8→L+2(+58%); H-7→L+2(+30%)
45	290.8	0.0026	H-1→L+5(+75%); H-2→L+6(+10%)
46	289.5	0.0000	H-8→L+3(+65%); H-7→L+3(+21%)
47	288.5	0.0012	H-2→L+4(+39%); H-1→L+7(+35%); H-8→L+2(+12%)
48	288.4	0.0000	H-1→L+6(+63%); H-2→L+5(+25%); H-8→L+3(+5%)
49	282.6	0.0000	H-4→L+8(+44%); H-3→L+9(+32%); H-5→L+9(+13%)
50	282.3	0.0360	H-4→L+9(+39%); H-3→L+8(+28%); H-5→L+8(+12%); H-7→L+2(6%)

51	281.6	0.0884	H-2→L+4(+30%); H-7→L+2(+27%); H-8→L+2(13%)
52	280.0	0.0378	H-1→L+7(+47%);H-2→L+4(+17%); H-7→L+2(+15%); H-9→L+3(+6%); H-8→L+2(+5%)
53	279.4	0.0000	H-7→L+3(+47%); H-8→L+3(22%); H-9→L+2(21%)
54	277.8	0.0000	H-9→L+2(+45%); H-2→L+7(+25%); H-6→L+2(5%)
55	276.5	0.0000	H-2→L+5(+54%); H-1→L+6(+34%); H-7→L+2(+5%)
56	275.5	0.0726	H-9→L+3(+42%); H-10→L(+27%); H-2→L+7(+15%)
57	274.7	0.0603	H-10→L(+41%); H-2→L+6(+25%); H-9→L+3(+9%); H-1→L+5(+8%)
58	274.3	0.0780	H-2→L+6(+52%); H-9→L+3(+18%); H-10→L(+10%); H-1→L+5(+5%)
59	273.8	0.0000	H-2→L+7(+61%); H-2→L+5(+12%); H-9→L+2(+9%)
60	272.6	0.0000	H-5→L+9(+35%); H-6→L+8(+27%); H-3→L+9(14%); H-9→L+8(+8%); H-7→L+9(+7%)
61	272.5	0.0019	H-5→L+8(+35%); H-6→L+9(+27%); H-3→L+8(14%); H-9→L+9(+8%); H-7→L+8(+7%)
62	270.7	0.0000	H-3→L+4(+73%); H-5→L+4(+13%); H-4→L+5(+7%); H-4→L+7(+6%)
63	270.3	0.0002	H-4→L+4(+81%); H-3→L+5(+7%)
64	268.1	0.0000	H-10→L+1(+69%); H-5→L+4(+15%)
65	267.8	0.0004	H-3→L+5(+38%); H-4→L+6(+32%); H-5→L+5(+13%); H-3→L+7(8%)
66	267.8	0.0000	H-4→L+5(+47%); H-3→L+6(+24%); H-5→L+6(+7%); H-4→L+7(+6%); H-3→L+4(5%)
67	267.0	0.0000	H-5→L+4(+52%); H-10→L+1(+16%); H-3→L+4(+7%)
68	262.1	0.0000	H-11→L(+76%)
69	261.2	0.1269	H-5→L+5(+16%); H-3→L+7(+14%); H-3→L+5(+13%); H→L+13(+8%); H-10→L+3 (+12%); H-6→L+4(+10%); H-11→L+1(7%)
70	260.3	0.0242	H→L+10(+78%); H-3→L+7(+9%)
71	259.9	0.0020	H-3→L+7(+48%);H-4→L+6(+12%)
72	259.6	0.0000	H-4→L+7(+80%); H-3→L+6(+8%)
73	258.6	0.0000	H→L+11(+94%)
74	258.3	0.0824	H-12→L(+60%); H-5→L+7(+13%); H-3→L+5(+5%)
75	258.3	0.1198	H-5→L+7(+30%); H-12→L(+23%); H-10→L+3(+9%); H-11→L+1(+6%);
76	257.8	0.0000	H-3→L+6(+41%); H-4→L+5(38%)
77	257.6	0.0009	H-4→L+6(+53%); H-5→L+5(22%); H-3→L+5(15%)
78	254.7	0.0000	H-10→L+2(+62%); H-2→L+8(+15%); H-1→L+9(+11%);
79	254.7	0.0000	H-2→L+8(+39%); H-1→L+9(+28%); H-10→L+2(+17%);
80	254.4	0.0099	H-2→L+9(+55%); H-1→L+8(37%)
81	254.0	0.0000	H-5→L+6(+40%); H-13→L(+20%); H-10→L+2(+10%); H-3→L+6(+8%);
82	253.1	0.0149	H-11→L+1(+28%); H-6→L+4(+25%); H-5→L+7(22%); H-3→L+7(+7%); H-6→L+6(+6%)
83	252.4	0.0208	H-11→L+1(+29%); H-6→L+4(+25%); H-5→L+5(19%); H-5→L+7(+7%); H-3→L+5(+6%)
84	251.7	0.0000	H-12→L+1(+60%); H-13→L(25%)
85	251.1	0.0000	H-13→L(+25%); H-12→L+1(+20%); H-6→L+5(+15%); H-5→L+6(+15%)
86	247.5	0.0000	H-6→L+5(+45%); H-6→L+7(+32%)
87	247.3	0.0017	H-6→L+6(+61%); H-13→L+1(+23%)
88	246.6	0.5826	H-10→L+3(+65%);H-6→L+4(+18%)
89	246.0	0.0000	H-6→L+7(+34%); H-14→L(+34%); H-6→L+5(8%)
90	244.9	0.0000	H-14→L(+45%); H-6→L+7(13%)
91	244.7	0.0226	H-13→L+1(+32%); H-15→L (+26%); H-14→L+1(+14%); H-6→L+6(10%); H-11→L+1 (+6%)
92	243.4	0.0079	H-15→L(+40%); H-13→L+1(26%); H-14→L+1(+11%); H-6→L+6(+6%); H-11→L+1(6%)
93	241.7	0.0000	H-7→L+4(+47%); H-8→L+4(+39%)
94	241.5	0.0000	H-17→L(+70%); H-18→L+1(+20%)
95	241.0	0.0083	H-18→L(+55%); H-17→L+1(+23%); H-8→L+5(+6%); H-16→L(+5%)
96	239.2	0.0000	H-12→L+2(+67%); H-8→L+4(13%); H-1→L+10(+5%)
97	238.8	0.0317	H-8→L+5(+27%); H-7→L+5(+26%); H-11→L+2(+11%); H-8→L+7(+8%); H-18→L(+7%); H-7→L+7(+6%);
98	238.0	0.2373	H-11→L+2(+40%); H-12→L+3(+28%); H-13→L+2(+10%)
99	237.9	0.0014	H-4→L+9(+49%); H-3→L+8(35%); H-5→L+8(13%)
100	237.9	0.0000	H-4→L+8(+50%); H-3→L+9(35%); H-5→L+9(14%)

Table S4. Calculated singlet excited-states transitions for the dimeric form of **1** with Pt···Pt distance of 3.362 Å and PF_6^- counterions in acetonitrile

No	nm	*f*	Assignment; H=HOMO, L=LUMO
1	510.9	0.0253	H→L(+97%)
2	489.1	0.0000	H→L+1(+97%)
3	425.7	0.0000	H-1→L(+71%); H→L+2(27%)
4	422.0	0.0000	H→L+2(+71%); H-1→L(+26%)
5	417.7	0.0003	H→L+3(+97%)
6	409.3	0.0473	H-2→L(+84%); H-1→L+1(+10%)
7	406.1	0.0065	H-1→L+1(+86%); H-2→L(12%)
8	391.8	0.0000	H-2→L+1(+42%); H-3→L(34%); H-5→L(+14%); H-6→L+1(+7%)
9	390.4	0.0000	H-3→L(+52%); H-2→L+1(+34%); H-4→L+1(+6%)
10	389.0	0.0002	H-4→L(+83%); H-3→L+1(+10%); H-5→L+1(+6%)
11	387.9	0.0000	H-5→L(+62%); H-2→L+1(20%); H-4→L+1(+10%)
12	382.1	0.0022	H-6→L(+40%); H-5→L+1(+31%); H-3→L+1(25%)
13	374.7	0.0232	H-1→L+2(+88%); H-2→L+3(+7%)
14	372.0	0.0000	H-1→L+3(+76%); H-2→L+2(+19%)
15	366.4	0.0033	H-3→L+1(+52%); H-5→L+1(+30%); H-4→L(16%)
16	365.7	0.0000	H-4→L+1(+81%); H-5→L(8%); H-3→L(7%)
17	356.3	0.0000	H-2→L+2(+79%); H-1→L+3(20%)
18	353.1	0.0051	H-2→L+3(+89%); H-1→L+2(8%)
19	347.6	0.0078	H-6→L(+55%); H-5→L+1(30%); H-3→L+1(+12%)
20	341.5	0.0000	H-6→L+1(+82%); H-5→L(9%)
21	334.9	0.0023	H-3→L+2(+64%); H-5→L+2(+20%); H-4→L+3(+14%)
22	334.5	0.0000	H-4→L+2(+76%); H-3→L+3(+17%)
23	330.9	0.0000	H-7→L(+41%); H-9→L(+41%)
24	329.0	0.0000	H-3→L+3(+51%); H-5→L+3(+26%); H-4→L+2(21%)
25	328.5	0.0089	H-4→L+3(+83%); H-3→L+2(12%)
26	326.6	0.0571	H→L+9(+47%); H-5→L+2(31%)
27	325.1	0.0000	H→L+8(+56%); H-7→L(18%)
28	322.8	0.0000	H-9→L(+50%); H-7→L(29%); H→L+8(8%)
29	321.9	0.0082	H→L+4(+88%); H-9→L+1(+6%)
30	320.8	0.0320	H-5→L+2(+31%); H→L+9(+28%); H-3→L+2(13%); H-9→L+1(+11%); H→L+4(6%)
31	319.9	0.0261	H-9→L+1(+52%); H-7→L+1(+24%); H→L+9(7%); H-5→L+2(6%)
32	318.0	0.0000	H→L+5(+54%); H-5→L+3(15%); H→L+7(10%); H→L+8(7%); H-3→L+3(+6%)
33	315.7	0.0000	H-5→L+3(+35%); H→L+5(+27%); H-3→L+3(14%); H→L+8(+8%)
34	312.6	0.1862	H→L+6(+50%); H-8→L(37%)
35	311.5	0.1937	H→L+6(+46%); H-8→L(+43%)
36	310.2	0.0000	H→L+7(+83%); H→L+5(+15%)
37	307.5	0.0762	H-7→L+1(+59%); H-9→L+1(24%); H-8→L(10%)
38	307.4	0.0000	H-6→L+2(+81%); H-8→L+2(+6%)
39	304.4	0.0000	H-8→L+1(+86%); H-7→L(8%)
40	303.7	0.0197	H-6→L+3(+80%); H-8→L+3(+6%)
41	297.0	0.0000	H-1→L+9(+56%); H-2→L+8(+39%)
42	296.9	0.0000	H-1→L+8(+56%); H-2→L+9(+38%)
43	292.2	0.0000	H-1→L+4(+85%); H-7→L+3(5%)
44	291.1	0.0146	H-9→L+2(+63%); H-7→L+2(+26%)
45	288.7	0.0009	H-1→L+5(+76%); H-2→L+6(+11%)
46	288.0	0.0000	H-9→L+3(+70%); H-7→L+3(+16%)
47	287.2	0.0036	H-1→L+7(+33%); H-2→L+4(+32%); H-9→L+2(+15%); H-7→L+2(8%)
48	286.5	0.0000	H-1→L+6(+64%); H-2→L+5(+25%)
49	282.5	0.0000	H-4→L+8(+44%); H-3→L+9(+32%); H-5→L+9(+13%)
50	282.2	0.0395	H-4→L+9(+37%); H-3→L+8(+27%); H-5→L+8(+12%); H-7→L+2(7%)

51	281.4	0.1041	H-7→L+2(+35%); H-2→L+4(+21%); H-9→L+2(11%); H-8→L+3(8%); H-4→L+9(+6%)
52	279.7	0.0000	H-7→L+3(+48%); H-8→L+2(26%); H-9→L+3(19%)
53	278.9	0.0053	H-1→L+7(+46%); H-2→L+4(32%)
54	277.6	0.0000	H-8→L+2(+47%); H-2→L+7(13%); H-7→L+3(+10%); H-6→L+2(8%)
55	276.0	0.0316	H-10→L(+54%); H-8→L+3(+30%); H-7→L+2(+6%)
56	274.9	0.0000	H-2→L+5(+48%); H-1→L+6(27%); H-2→L+7(15%)
57	274.5	0.1854	H-8→L+3(+36%); H-10→L(30%); H-1→L+7(+10%); H-6→L+3(6%)
58	272.8	0.0097	H-2→L+6(+72%); H-1→L+5(11%)
59	272.7	0.0000	H-2→L+7(+61%); H-2→L+5(+20%)
60	272.3	0.0000	H-5→L+9(+35%); H-6→L+8(+26%); H-3→L+9(14%); H-8→L+8(+8%); H-7→L+9(+8%)
61	272.1	0.0006	H-5→L+8(+32%); H-6→L+9(+24%); H-3→L+8(12%); H-2→L+6(+9%); H-8→L+9(+7%); H-7→L+8(+7%)
62	269.5	0.0000	H-3→L+4(+74%); H-5→L+4(+13%); H-4→L+7(+7%)
63	269.1	0.0002	H-4→L+4(+83%); H-3→L+7(+6%); H-3→L+5(+5%)
64	268.2	0.0000	H-10→L+1(+86%)
65	266.6	0.0004	H-3→L+5(+40%); H-4→L+6(+32%); H-5→L+5(+13%); H-3→L+7(8%)
66	266.6	0.0000	H-4→L+5(+47%); H-3→L+6(+22%); H-5→L+4(+10%); H-5→L+6(+8%); H-3→L+4(5%)
67	266.0	0.0000	H-5→L+4(+59%); H-3→L+4(9%); H-4→L+5(6%); H-4→L+7(+5%)
68	262.2	0.0000	H-11→L(+77%)
69	260.3	0.1249	H-3→L+7(+18%); H-10→L+3(+15%); H-5→L+5(14%); H-3→L+5(+12%); H-6→L+4(11%); H→L+10(8%); H-11→L+1(7%)
70	259.4	0.0146	H→L+10(+75%); H-3→L+7(+11%); H-12→L(+5%)
71	259.1	0.0036	H-3→L+7(+42%); H-5→L+7(+11%); H-4→L+6(+11%); H→L+10(10%); H-5→L+5(+9%); H-4→L+4(5%)
72	258.8	0.0000	H-4→L+7(+80%); H-3→L+6(+8%)
73	257.9	0.1202	H-12→L(+73%)
74	257.7	0.0511	H-5→L+7(+36%); H-11→L+1(10%); H-10→L+3(9%); H-3→L+5(+9%); H-12→L(7%); H-5 → L+5(7%); H-6→L+4(+5%)
75	257.5	0.0000	H→L+11(+94%)
76	256.7	0.0000	H-3→L+6(+42%); H-4→L+5(39%); H-5→L+6(+8%)
77	256.4	0.0012	H-4→L+6(+54%); H-3→L+5(19%); H-5→L+5(18%)
78	255.0	0.0000	H-10→L+2(+88%)
79	254.2	0.0000	H-2→L+8(+55%); H-1→L+9(39%)
80	254.0	0.0112	H-2→L+9(+54%); H-1→L+8(37%)
81	253.3	0.0000	H-5→L+6(+42%); H-13→L(+30%); H-3→L+6(7%)
82	252.6	0.0248	H-11→L+1(+39%); H-5→L+7(+17%); H-6→L+4(11%); H-5→L+5(9%); H-6→L+6(+5%); H-3→L+7(5%)
83	251.6	0.0194	H-6→L+4(+35%); H-5→L+5(17%); H-5→L+7(15%); H-11→L+1(+14%); H-3→L+7(+5%)
84	251.2	0.0000	H-12→L+1(+62%); H-13→L(23%)
85	250.6	0.0000	H-13→L(+23%); H-5→L+6(20%); H-12→L+1(+19%); H-6→L+5(+8%); H-3→L+6(+6%)
86	246.7	0.0000	H-6→L+5(+51%); H-6→L+7(+29%)
87	246.6	0.5507	H-10→L+3(+59%); H-6→L+4(+19%); H-11→L+2(+5%)
88	246.5	0.0307	H-6→L+6(+53%); H-13→L+1(+27%)
89	245.5	0.0000	H-14→L(+40%); H-6→L+7(+32%); H-6→L+5(6%); H-15→L+1(+5%)
90	244.5	0.0000	H-14→L(+38%); H-6→L+7(18%); H-6→L+5(+14%); H-13→L(7%)
91	244.4	0.0224	H-13→L+1(+34%); H-15→L (+22%); H-6→L+6(15%); H-14→L+1(+12%); H-11→L+1 (+6%)
92	243.2	0.0062	H-15→L(+44%); H-13→L+1(21%); H-14→L+1(+13%); H-6→L+6(+6%)
93	241.4	0.0000	H-17→L(+70%); H-18→L+1(+19%)
94	240.7	0.0102	H-18→L(+58%); H-17→L+1(+24%); H-15→L(7%)
95	240.5	0.0000	H-7→L+4(+47%); H-9→L+4(+33%); H-1→L+10(+7%); H-12→L+2(+6%)
96	238.8	0.0000	H-12→L+2(+62%); H-9→L+4(15%); H-11→L+3(+11%)
97	238.3	0.2923	H-11→L+2(+59%); H-9→L+5(+6%)
98	237.8	0.0065	H-4→L+9(+49%); H-3→L+8(35%); H-5→L+8(13%)
99	237.8	0.0000	H-4→L+8(+50%); H-3→L+9(36%); H-5→L+9(14%)
100	237.4	0.1045	H-12→L+3(+54%); H-13→L+2(+10%); H-11→L+2(9%); H-7→L+5(+6%)

Table S5. Calculated singlet excited-states transitions for the trimeric form of **1**-MeCN in the absence of PF_6^- counterions

No	nm	*f*	Assignment; H=HOMO, L=LUMO
1	575.6	0.0294	H→L(+95%)
2	504.0	0.0170	H→L+2(+90%)
3	503.7	0.0002	H→L+1(+92%)
4	493.8	0.0006	H-1→L(+96%)
5	471.7	0.0022	H-2→L(+93%)
6	463.2	0.0003	H→L+3(+93%)
7	448.5	0.0013	H-3→L(+90%); H-4→L+1(5%)
8	445.2	0.0019	H-4→L(+85%); H-3→L+1(8%)
9	439.4	0.0316	H-1→L+2(+63%); H-2→L+1(+22%)
10	439.2	0.0025	H-1→L+1(+64%); H-2→L+2(+23%)
11	430.7	0.0016	H→L+4(+90%)
12	429.0	0.0000	H→L+5(+88%)
13	424.1	0.0068	H-5→L(+52%); H-3→L+2(23%); H-4→L+1(18%)
14	423.8	0.0056	H-5→L(+40%); H-3→L+2(+28%); H-4→L+1(+23%)
15	423.4	0.0003	H-4→L+2(+45%); H-3→L+1(+43%); H-4→L(+8%)
16	414.4	0.0032	H-1→L+3(+78%); H-2→L+1(15%)
17	407.8	0.0003	H-2→L+2(+64%); H-1→L+1(25%)
18	406.3	0.0019	H-2→L+1(+50%); H-1→L+2(24%); H-1→L+3(+18%)
19	398.8	0.0001	H-1→L+4(+58%); H-2→L+5(+22%); H-2→L+3(+15%)
20	397.4	0.0179	H-1→L+5(+62%); H-2→L+4(+34%)
21	394.1	0.0017	H-2→L+3(+59%); H-5→L+1(25%); H-2→L+5(7%)
22	393.3	0.0024	H-6→L(+75%); H-10→L(+9%); H-5→L+2(+7%)
23	392.6	0.0000	H-5→L+1(+71%); H-2→L+3(+18%)
24	390.9	0.0001	H-5→L+2(+87%); H-6→L(5%)
25	389.4	0.0002	H-9→L(+71%); H-8→L(+24%)
26	382.8	0.0002	H-6→L+1(+31%); H-8→L+2(+22%);H-8→L(20%); H-9→L(+13%); H-7→L+1(6%)
27	381.6	0.0028	H-7→L(+40%); H-8→L+1(+23%); H-6→L+2(+21%)
28	380.2	0.0013	H-3→L+3(+61%); H-3→L+2(+19%); H-4→L+1(15%)
29	378.8	0.0015	H-4→L+3(+49%); H-4→L+2(+29%); H-3→L+1(20%)
30	373.9	0.0003	H-7→L(+48%); H-6→L+2(17%); H-10→L(14%); H-8→L+1(9%)
31	373.4	0.0004	H-4→L+1(+36%); H-3→L+3(+33%); H-3→L+2(26%)
32	372.7	0.0012	H-4→L+3(+48%); H-3→L+1(+26%); H-4→L+2(22%)
33	367.4	0.0045	H-5→L+3(+81%); H-3→L+5(5%); H-4→L+4(5%)
34	366.8	0.0001	H-3→L+4(+53%); H-4→L+5(+44%)
35	366.6	0.0005	H-3→L+5(+46%); H-4→L+4(+41%); H-5→L+3(+10%)
36	364.1	0.0027	H-8→L(+52%); H-6→L+1(+16%); H-8→L+2(+14%); H-9→L(+13%)
37	362.5	0.0004	H-2→L+4(+62%); H-1→L+5(34%)
38	362.1	0.0001	H-2→L+5(+62%); H-1→L+4(30%)
39	359.0	0.0016	H→L+6(+41%); H→L+7(+39%); H-7→L+1(10%)
40	358.3	0.0008	H→L+6(+57%); H→L+7(25%); H-7→L+1(+10%)
41	356.5	0.0021	H-10→L(+53%); H-7→L+2(+15%); H-6→L(13%); H-8→L+1(7%)
42	356.5	0.0020	H-7→L+1(+48%); H→L+7(+29%); H-6→L+1(+13%)
43	355.8	0.0032	H-7→L+2(+52%); H-6→L+2(+24%); H-10→L(11%)
44	350.1	0.0025	H-5→L+4(+91%)
45	349.2	0.0025	H-9→L+1(+58%); H-5→L+5(+20%); H-8→L+1(+12%)
46	348.7	0.0004	H-9→L+2(+76%); H-8→L+2(+15%)
47	348.7	0.0012	H-5→L+5(+69%); H-9→L+1(21%)
48	345.3	0.0032	H→L+12(+78%)
49	336.8	0.0000	H-4→L+4(+51%); H-3→L+5(47%)
50	336.7	0.0000	H-4→L+5(+54%); H-3→L+4(44%)

51	335.3	0.0028	H-6→L+2(+32%); H-8→L+1(28%); H-7→L+2(14%); H-9→L+1(+11%); H-10→L+2(+8%)
52	335.1	0.0000	H-8→L+2(+32%); H-6→L+1(30%); H-7→L+1(+13%); H-9→L+2(12%); H-10→L+1(10%)
53	332.2	0.0069	H-6→L+3(+46%); H-7→L+3(+31%); H-11→L(10%)
54	329.7	0.0040	H-11→L(+77%); H-7→L+3(+7%)
55	329.3	0.0005	H-9→L+3(+72%); H-8→L+3(+24%)
56	328.2	0.0001	H-1→L+6(+56%); H-1→L+7(+32%); H→L+8(7%)
57	325.0	0.0008	H→L+9(+44%); H-1→L+7(+24%); H→L+8(+17%)
58	324.2	0.0009	H-12→L(+74%); H-6→L+4(+11%)
59	323.8	0.0061	H-1→L+7(+40%); H-1→L+6(26%); H→L+9(15%); H-6→L+5(+6%)
60	323.6	0.0147	H→L+8(+37%); H-7→L+3(21%); H-6→L+3(+12%); H-1→L+6(+8%); H-6→L+5(+6%)
61	323.2	0.0013	H-6→L+4(+28%); H-12→L(17%); H→L+10(+17%); H-8→L+3(+6%)
62	322.8	0.0060	H-7→L+3(+29%); H-6→L+3(20%); H→L+8(+17%); H→L+9(13%); H-10→L+2(+6%)
63	321.1	0.0006	H→L+11(+37%); H-10→L+1(+23%); H-7→L+4(13%); H-8→L+3(+7%)
64	320.2	0.0013	H-10→L+1(+37%); H→L+11(27%); H→L+10(6%)
65	320.0	0.0108	H-10→L+2(+66%); H-8→L+1(+8%)
66	319.2	0.0025	H→L+10(+52%); H-8→L+3(13%); H-10→L+1(+10%); H-6→L+4(8%)
67	318.9	0.0065	H-6→L+5(+35%); H→L+9(+15%); H→L+8(8%); H-10→L+2(7%); H→L+14(6%)
68	318.2	0.0000	H-8→L+3(+30%); H-9→L+3(10%); H-10→L+1(10%); H-6→L+4(9%); H→L+10(+9%); H→L+11(8%); H-7→L+4(8%)
69	317.8	0.0004	H-2→L+6(+28%); H-2→L+7(+17%); H→L+11(+10%); H-7→L+4(+9%); H-8→L+3(+9%); H→L+10(+7%)
70	316.6	0.0131	H-7→L+5(+39%); H→L+14(+19%); H-8→L+4(8%)
71	316.4	0.0010	H-7→L+4(+22%); H-2→L+6(21%); H→L+13(+15%); H-2→L+7(14%); H→L+11(+7%)
72	315.4	0.0009	H-9→L+4(+76%); H-8→L+4(+18%)
73	315.2	0.0004	H-13→L(+44%); H-11→L+2(15%); H-12→L+1(10%); H-11→L(6%)
74	314.8	0.0025	H-9→L+5(+76%); H-8→L+5(+18%)
75	313.8	0.0000	H-2→L+7(+44%); H-2→L+6(33%); H-11→L+1(+7%); H-12→L+2(+5%)
76	311.8	0.0002	H-11→L+1(+31%); H-12→L+2(+19%); H→L+13(+14%); H-2→L+7(6%)
77	311.4	0.0007	H→L+13(+22%); H-7→L+4(16%); H-11→L+1(11%); H-2→L+7(+8%); H-12→L+2(7%); H-14→L(+6%); H-1→L+14(+5%)
78	310.9	0.0082	H→L+14(+37%); H-7→L+5(19%); H-1→L+13(+7%); H-8→L+4(+7%); H-6→L+5(+6%)
79	308.3	0.0008	H-14→L(+75%)
80	307.4	0.2949	H-11→L+2(+30%); H-13→L(+25%); H-12→L+1(+19%)
81	305.0	0.0001	H-3→L+6(+54%); H-3→L+7(+37%)
82	304.5	0.0002	H-2→L+14(+29%); H-1→L+13(+24%); H-3→L+6(7%); H-6→L+5(7%)
83	304.4	0.0000	H-1→L+9(+29%);H-1→L+14(+19%);H-2→L+13(+18%);H-2→L+10(8%);H-2→L+11 (+7%)
84	304.2	0.0000	H-1→L+9(+34%); H-1→L+14(17%); H-2→L+13(16%); H-2→L+11(+14%)
85	303.8	0.0064	H-8→L+4(+24%); H-6→L+5(18%); H-1→L+10(+12%); H-7→L+5(+12%); H-9→L+4(10%)
86	303.7	0.0010	H-8→L+5(+27%); H-6→L+4(20%); H-1→L+8(+15%); H-7→L+4(+11%); H-9→L+5(11%); H-2→L+10(+5%)
87	303.7	0.0036	H-1→L+11(+36%); H-2→L+9(+32%); H-1→L+10(11%)
88	303.2	0.0002	H-4→L+6(+59%); H-4→L+7(+35%)
89	302.4	0.0133	H-5→L+6(+52%); H-10→L+3(+25%)
90	301.6	0.0000	H-1→L+8(+40%); H-8→L+5(17%); H-2→L+10(+10%)
91	301.2	0.0057	H-3→L+7(+35%); H-3→L+6(22%); H-2→L+8(+11%); H-1→L+10(+10%); H-1→L+11 (7%)
92	300.9	0.0169	H-3→L+7(+18%); H-1→L+10(16%); H-2→L+8(16%); H-3→L+6(11%); H-1→L+11(10%); H-8→L+4(+7%)
93	299.8	0.0000	H-5→L+12(+69%); H-1→L+12(+13%); H-7→L+12(7%)
94	299.3	0.0001	H-4→L+7(+59%); H-4→L+6(36%)
95	299.2	0.0013	H-5→L+7(+84%)
96	297.6	0.0048	H-5→L+6(+19%); H-12→L+1(+19%); H-11→L+2(16%); H-10→L+3(14%); H-13→L+2(7%); H-15→L(6%)
97	296.9	0.0002	H-12→L+2(+50%); H-11→L+1(35%); H-13→L+1(9%)
98	296.6	0.0099	H-12→L+1(+28%); H-11→L+2(24%); H-10→L+3(14%); H-5→L+6(12%); H-13→L+3(6%)
99	293.8	0.0000	H-3→L+14(+45%); H-4→L+13(+38%); H-4→L+15(5%)
100	293.6	0.0410	H-4→L+14(+42%); H-3→L+13(+38%); H-3→L+15(5%)

Table S6. Calculated singlet excited-states transitions for the trimeric form of **1**-MeCN in the presence of PF_6^- counterions

No	nm	*f*	Assignment; H=HOMO, L=LUMO
1	567.7	0.0001	H→L(+79%); H-1→L+1(+20%)
2	567.5	0.0000	H-1→L(+78%); H→L+1(+21%)
3	553.0	0.0000	H-2→L(+78%); H-3→L+1(+20%)
4	553.0	0.0001	H-3→L(+78%); H-2→L+1(+20%)
5	549.9	0.0454	H-6→L(+91%)
6	545.5	0.0000	H→L+1(+76%); H-1→L(21%)
7	545.4	0.0000	H-1→L+1(+70%); H→L(18%); H-4→L(7%)
8	544.7	0.0000	H-4→L(+69%); H-5→L+1(+20%); H-1→L+1(+7%)
9	544.4	0.0000	H-5→L(+74%); H-4→L+1(+24%)
10	538.6	0.0003	H-6→L+1(+94%)
11	531.9	0.0000	H-2→L+1(+77%); H-3→L(20%)
12	531.9	0.0001	H-3→L+1(+77%); H-2→L(20%)
13	522.6	0.0000	H-4→L+1(+72%); H-5→L(24%)
14	522.3	0.0000	H-5→L+1(+74%); H-4→L(21%)
15	519.9	0.0010	H-6→L+2(+92%)
16	514.8	0.0000	H→L+2(+97%)
17	514.6	0.0000	H-1→L+2(+97%)
18	502.7	0.0006	H-2→L+2(+97%)
19	502.7	0.0001	H-3→L+2(+96%)
20	495.0	0.0000	H-4→L+2(+96%)
21	494.5	0.0000	H-5→L+2(+96%)
22	483.6	0.0000	H→L+3(+64%); H-1→L+4(+35%)
23	483.5	0.0001	H-1→L+3(+62%); H→L+4(+37%)
24	473.0	0.0000	H-2→L+3(+63%); H-3→L+4(+36%)
25	473.0	0.0000	H-3→L+3(+62%); H-2→L+4(+36%)
26	471.3	0.0000	H→L+4(+62%); H-1→L+3(37%)
27	471.2	0.0000	H-1→L+4(+64%); H→L+3(35%)
28	466.4	0.0000	H-4→L+3(+63%); H-5→L+4(+35%)
29	466.3	0.0000	H-5→L+3(+59%); H-4→L+4(+39%)
30	464.7	0.0009	H-6→L+3(+89%)
31	463.0	0.0149	H-7→L(+74%); H-9→L(7%); H-8→L+1(+6%)
32	462.2	0.0000	H-6→L+4(+82%)
33	461.1	0.0000	H-2→L+4(+63%); H-3→L+3(36%)
34	461.1	0.0000	H-3→L+4(+62%); H-2→L+3(35%)
35	459.2	0.0016	H-7→L+1(+35%); H-10→L(25%); H-9→L+1(23%); H-8→L(+14%)
36	459.0	0.0013	H-9→L(+49%); H-10→L+1(+36%)
37	457.8	0.0023	H-7→L+1(+33%); H-10→L(+23%); H-9→L+1(+18%); H-8→L(+11%); H-6→L+4(9%)
38	453.7	0.0000	H-4→L+4(+60%); H-5→L+3(39%)
39	453.6	0.0000	H-5→L+4(+63%); H-4→L+3(36%)
40	442.5	0.0082	H-7→L+2(+67%); H-11→L(17%); H-8→L+1(+12%)
41	438.8	0.0241	H-11→L(+71%); H-8→L+1(+10%); H-7→L+2(+9%)
42	435.5	0.0006	H-11→L+1(+46%); H-8→L(+36%); H-7→L+1(7%); H-8→L+2(6%)
43	431.6	0.0001	H-11→L+1(+44%); H-8→L(23%); H-7→L+1(+16%); H-8→L+2(+10%)
44	424.3	0.0000	H→L+5(+99%)
45	424.1	0.0000	H-1→L+5(+99%)
46	422.1	0.0019	H-8→L+1(+62%); H-7→L+2(17%); H-7→L(13%)
47	418.7	0.0003	H-7→L+3(+65%); H-8→L+4(+21%); H-8→L+2(+8%)
48	416.8	0.0205	H-7→L+4(+66%); H-8→L+3(+29%)
49	416.2	0.0003	H-2→L+5(+98%)
50	416.2	0.0000	H-3→L+5(+99%)

51	414.5	0.0013	H-9→L+2(+57%); H-10→L+1(+18%); H-9→L(18%)
52	412.6	0.0000	H-8→L+2(+66%); H-8→L(+7%); H-8→L+4(6%); H-7→L+3(6%)
53	411.8	0.0002	H-10→L+2(+45%); H-10→L(25%); H-9→L+1(+19%); H-8→L+2(6%)
54	411.8	0.0001	H-4→L+5(+98%)
55	411.4	0.0000	H-5→L+5(+98%)
56	410.9	0.0021	H-11→L+2(+83%); H-9→L+2(+6%)
57	409.0	0.0010	H-6→L+5(+97%)
58	397.8	0.0014	H-19→L(+86%); H-19→L+2(7%)
59	395.9	0.0000	H-10→L+1(+36%); H-9→L+2(32%); H-9→L(18%)
60	395.5	0.0017	H-16→L(+59%); H-16→L+2(7%)
61	395.2	0.0000	H-10→L+2(+42%); H-9→L+1(28%); H-10→L(+18%); H-9→L+3(+6%)
62	391.9	0.0000	H-9→L+4(+50%); H-10→L+3(+45%)
63	391.8	0.0002	H-9→L+3(+50%); H-10→L+4(+41%)
64	388.2	0.0007	H-16→L+1(+46%); H-26→L(+20%); H-25→L+1(+15%)
65	388.0	0.0007	H-19→L+1(+89%); H-18→L+1(5%)
66	386.4	0.0012	H-11→L+3(+87%); H-8→L+4(+6%)
67	384.2	0.0005	H-11→L+4(+74%); H-8→L+3(+12%)
68	381.4	0.0022	H-16→L+2(+31%); H-26→L+1(+24%); H-25→L(+22%)
69	379.1	0.0004	H-8→L+3(+53%); H-7→L+4(25%); H-11→L+4(15%)
70	378.6	0.0003	H-8→L+4(+63%); H-7→L+3(25%); H-11→L+3(6%)
71	376.7	0.0007	H-19→L+2(+81%); H-19→L(+7%)
72	375.0	0.0004	H-12→L(+77%); H-13→L+1(+20%)
73	374.7	0.0000	H-13→L(+72%); H-12→L+1(+24%)
74	373.5	0.0016	H-16→L+1(+27%); H-26→L(20%); H-22→L+1(19%); H-25→L+1(13%)
75	373.3	0.0000	H-14→L(+71%); H-15→L+1(+18%)
76	373.2	0.0014	H-22→L(+41%); H-16→L+2(17%); H-16→L(7%); H-14→L (+6%);H-26→L+1(+6%)
77	372.8	0.0001	H-15→L(+68%); H-14→L+1(+23%)
78	365.0	0.0010	H-7→L+5(+77%); H-22→L(7%)
79	364.5	0.0029	H-22→L(+24%); H-7→L+5(+20%); H-16→L+2(+16%); H-16→L(+12%); H-25→L(8%)
80	364.5	0.0000	H-12→L+1(+50%); H-22→L+1(18%); H-13→L(15%)
81	364.2	0.0000	H-13→L+1(+74%); H-12→L(20%)
82	364.1	0.0000	H-22→L+1(+33%); H-12→L+1(+21%); H-16→L+1(+8%); H-13→L(8%); H-14→L+1 (7%); H-23→L+1(+5%)
83	362.5	0.0000	H-14→L+1(+62%); H-15→L(23%)
84	362.2	0.0000	H-15→L+1(+74%); H-14→L(19%)
85	360.0	0.0003	H-17→L(+76%); H-18→L+1(+16%)
86	359.2	0.0000	H-18→L(+65%); H-17vL+1(+25%)
87	358.9	0.0002	H-10→L+3(+51%); H-9→L+4(43%)
88	358.7	0.0001	H-10→L+4(+54%); H-9→L+3(39%)
89	357.7	0.0005	H-20→L(+76%); H-21→L+1(+15%)
90	357.5	0.0004	H-6→L+6(+94%)
91	357.2	0.0000	H→L+6(+96%)
92	357.0	0.0000	H-21→L(+46%); H-1→L+6(31%); H-20→L+1(+16%)
93	357.0	0.0000	H-1→L+6(+63%); H-21→L(+23%); H-20→L+1(+8%)
94	351.4	0.0001	H-2→L+6(+86%); H-12→L+2(9%)
95	351.4	0.0000	H-3→L+6(+87%)
96	350.7	0.0001	H-12→L+2(+85%); H-2→L+6(+9%)
97	350.5	0.0002	H-17→L+1(+52%); H-18→L(21%); H-13→L+2(6%); H-3→L+6(6%)
98	350.3	0.0001	H-13→L+2(+77%)
99	350.1	0.0002	H-1→L+9(+37%); H→L+10(24%); H→L+8(+19%); H-1→L+7(+11%)
100	350.0	0.0000	H→L+9(+35%); H-1→L+10(22%); H-1→L+8(+17%); H→L+7(+11%); H-13→L+2(8%)

Table S7. Calculated singlet excited-states transitions for the trimeric form of **1** in the presence of PF_6^- counterions

No	nm	*f*	Assignment; H=HOMO, L=LUMO
1	607.7	0.0000	H→L(+98%)
2	597.1	0.0000	H-1→L(+99%)
3	571.5	0.0000	H→L+1(+93%); H→L+2(6%)
4	561.4	0.0002	H-1→L+1(+93%); H-1→L+2(7%)
5	558.1	0.0000	H-2→L+1(+92%); H-2→L(6%)
6	551.6	0.0000	H-3→L+1(+91%); H-3→L(7%)
7	547.9	0.0000	H-2→L(+93%); H-2→L+1(+6%)
8	544.3	0.0000	H→L+2(+92%); H→L+1(+6%)
9	542.2	0.0001	H-3→L(+93%); H-3→L+1(+6%)
10	535.7	0.0000	H-4→L(+97%)
11	535.4	0.0005	H-1→L+2(+90%); H-1→L+1(+6%)
12	519.4	0.0000	H-2→L+2(+95%)
13	513.8	0.0000	H-5→L+1(+92%); H-5→L(6%)
14	513.0	0.0005	H-3→L+2(+96%)
15	508.0	0.0000	H-4→L+1(+92%); H-4→L+2(7%)
16	504.4	0.0000	H-5→L(+93%); H-5→L+1(+6%)
17	497.5	0.0093	H-6→L+1(+47%); H-8→L+1(42%)
18	487.0	0.0001	H-4→L+2(+91%); H-4→L+1(+7%)
19	482.8	0.0000	H→L+4(+96%)
20	479.6	0.0103	H-7→L(+52%); H-9→L(29%); H-6→L(+14%)
21	478.8	0.0003	H-5→L+2(+96%)
22	476.0	0.0000	H-1→L+4(+96%)
23	473.8	0.0177	H-8→L+1(+47%); H-6→L+1(+34%)
24	471.0	0.0060	H-9→L(+52%); H-6→L(+30%); H-7→L(+6%)
25	468.7	0.0000	H→L+3(+96%)
26	468.5	0.0056	H-7→L(+32%); H-6→L(22%); H-6→L+2(+17%); H-9→L(+12%)
27	465.5	0.0037	H-6→L+2(+35%); H-10→L+1(+26%); H-6→L(+18%); H-8→L+2(7%)
28	464.4	0.0019	H-10→L+1(+56%); H-6→L+2(23%)
29	461.8	0.0000	H-1→L+3(+95%)
30	460.8	0.0000	H-2→L+3(+95%)
31	456.5	0.0000	H-3→L+3(+95%)
32	456.1	0.0024	H-8→L(+89%)
33	445.7	0.0063	H-7→L+2(+42%); H-7→L+1(42%)
34	444.5	0.0000	H-2→L+4(+96%)
35	440.8	0.0000	H-3→L+4(+96%)
36	438.2	0.0076	H-8→L+2(+76%); H-6→L+2(+13%)
37	435.8	0.0001	H-4→L+4(+96%)
38	433.4	0.0040	H-7→L+2(+47%); H-7→L+1(+28%); H-11→L+1(+15%)
39	432.4	0.0000	H→L+5(+98%)
40	430.3	0.0002	H-5→L+3(+95%)
41	427.0	0.0002	H-1→L+5(+98%)
42	424.9	0.0004	H-4→L+3(+91%)
43	424.3	0.0113	H-11→L+1(+58%); H-7→L+1(14%); H-6→L+3(+8%)
44	420.3	0.0003	H-11→L(+68%); H-10→L(9%); H-6→L(+6%); H-22→L(+6%)
45	418.1	0.0095	H-6→L+3(+75%); H-11→L+1(7%)
46	415.4	0.0000	H-2→L+5(+93%)
47	415.3	0.0000	H-5→L+4(+92%)
48	412.1	0.0012	H-10→L(+48%); H-10→L+2(37%); H-11→L(+6%)
49	410.5	0.0005	H-3→L+5(+96%)
50	409.7	0.0007	H-10→L+2(+55%); H-10→L(+36%)

51	408.9	0.0005	H-9→L+2(+58%); H-9→L+1(35%)
52	406.7	0.0088	H-7→L+4(+75%); H-6→L+4(+11%)
53	402.2	0.0042	H-8→L+3(+88%)
54	400.4	0.0051	H-11→L+2(+77%)
55	396.5	0.0000	H-9→L+1(+53%); H-9→L+2(+36%)
56	396.1	0.0007	H-4→L+5(+98%)
57	394.6	0.0014	H-16→L+1(+77%); H-16→L+2(6%); H-16→L(6%)
58	392.0	0.0043	H-22→L(+32%); H-6→L+4(22%); H-24→L(+13%); H-16→L(9%)
59	391.5	0.0005	H-16→L(+77%); H-6→L+4(6%)
60	389.5	0.0006	H-6→L+4(+45%); H-22→L(+18%); H-24→L(+8%); H-7→L+4(8%); H-11→L(6%)
61	388.7	0.0001	H-5→L+5(+98%)
62	386.5	0.0021	H-17→L(+41%); H-25→L(20%); H-12→L(10%)
63	382.6	0.0020	H-10→L+3(+58%);H-7→L+3(11%); H-8→L+4(+6%)
64	382.6	0.0021	H-16→L+2(+21%); H-17vL+1(16%); H-10→L+3(12%); H-22→L+1(+9%); H-23→L+1(8%); H-24→L+1(7%)
65	382.0	0.0079	H-8→L+4(+66%); H-10→L+3(10%); H-9→L+4(+5%)
66	380.9	0.0022	H-16→L+2(+62%) H-16->L+1(+7%) ;H-22→L+1(6%)
67	379.0	0.0008	H-9→L+4(+85%)
68	377.4	0.0015	H-17→L+2(+27%); H-22→L+1(12%); H-24→L+1(+10%); H-23→L+1(+7%); H-17→L+1(5%)
69	377.0	0.0003	H-13→L(+42%); H-12→L(+41%); H-25→L(7%)
70	374.6	0.0025	H-7→L+3(+59%); H-11→L+3(+15%); H-10→L+3(+12%)
71	374.3	0.0000	H→L+6(+96%)
72	373.5	0.0010	H-15→L(+33%); H-25→L(22%); H-14→L(+15%); H-13→L(8%)
73	372.9	0.0000	H-12→L+1(+38%); H-13→L+1(38%); H-15→L(+7%)
74	370.4	0.0001	H-1→L+6(+93%)
75	369.8	0.0004	H-14→L+1(+59%); H-15→L(+10%); H-15→L+1(6%)
76	369.4	0.0008	H-15→L(+19%); H-17→L(+18%); H-13→L(+15%); H-25→L(+12%); H-14→L+1(11%); H-12→L(6%)
77	368.2	0.0066	H-6→L+5(+79%); H-7→L+5(6%)
78	367.3	0.0006	H-12→L(+29%); H-13→L(28%); H-17→L(+15%); H-25→L(+6%)
79	366.7	0.0002	H-17→L+1(+24%); H-17→L+2(+14%); H-15→L+1(13%); H-13→L+1(10%)
80	364.5	0.0016	H-11→L+3(+72%); H-7→L+3(13%)
81	364.3	0.0000	H-14→L(+64%); H-15→L(17%); H-17→L(+6%)
82	362.7	0.0001	H-13→L+1(+36%); H-12→L+1(+32%); H-17→L+1(+8%); H-15→L+1(7%); H-12→L+2(6%)
83	360.3	0.0000	H→L+7(+62%); H→L+8(35%)
84	358.0	0.0004	H-15→L+1(+53%); H-17→L+1(+19%); H-14→L+1(+10%); H-15→L+2(7%)
85	356.5	0.0002	H-1→L+7(+61%); H-1→L+8(36%)
86	356.3	0.0047	H-8→L+5(+47%); H-7→L+5(44%)
87	355.5	0.0003	H-11→L+4(+61%); H-7→L+5(9%); H-8→L+5(8%); H-10→L+4(6%); H-6→L+4(+6%)
88	354.8	0.0046	H-8→L+5(+37%); H-7→L+5(+32%); H-11→L+4(+14%); H-6→L+5(+9%)
89	354.7	0.0004	H-13→L+2(+53%); H-12→L+2(35%)
90	353.9	0.0001	H→L+10(+57%); H→L+9(+14%); H→L+7(+14%); H→L+8(+11%)
91	353.5	0.0000	H-2→L+6(+96%)
92	352.8	0.0001	H-12→L+2(+39%); H-13→L+2(+37%)
93	351.9	0.0001	H-19→L(+39%); H→L+8(28%); H→L+7(12%); H-18→L(+10%)
94	351.6	0.0000	H-19→L(+33%); H→L+8(+25%); H→L+10(17%); H→L+7(+10%); H-18→L(+8%)
95	351.5	0.0003	H-14→L+2(+68%); H-15→L+2(19%); H-3→L+6(+5%)
96	351.1	0.0000	H-3→L+6(+92%)
97	350.0	0.0000	H-1→L+10(+55%); H-1→L+7(+15%); H-1→L+9(+14%); H-1→L+8(+13%)
98	349.1	0.0001	H-10→L+4(+85%); H-11→L+4(+9%)
99	348.8	0.0000	H-2→L+7(+83%); H-2→L+9(+7%); H-2→L+8(5%)
100	348.2	0.0007	H-15→L+2(+58%); H-17→L+2(+10%); H-14→L+2(+10%); H-15→L+1(+6%)