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Supporting Information

A Luminescent Trinuclear Platinum(II) Pt_3C_2 System Having a "Naked" $C^{\circ}C^{2-}$ Ligand Swapping amongst Three Unsupported Platinum(II) Moieties

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Synthesis and Characterization

[{Pt(^{t}Bu$_3$-trpy)}$_3$(μ$_3$-?^{1},?^{2}-C≡C-)](PF$_6$)$_4$ (**1**·PF$_6$) was obtained as a by-product from the treatment of the dinuclear alkynylplatinum(II) terpyridyl precursor, [Pt(^{t}Bu$_3$-trpy)(C≡C)Pt(^{t}Bu$_3$-trpy)](OTf)$_2$, with an excess amount of [Cu(MeCN)$_4$]PF$_6$ in acetone. After removal of solvent under vacuum, the solid residue was washed with THF and yellowish-orange crystals of **1**·PF$_6$ were obtained after recrystallization from dichloromethane/*n*-hexane. X-Ray quality crystals can be obtained from slow vapor diffusion of *n*-hexane into a solution of **1**·PF$_6$ in acetone. Yield: 10 %. Positive ESI-MS: m/z 2250 [*M*–PF$_6$]$^+$, 1052 [*M*–2(PF$_6$)]$^{2+}$; elemental analysis (%) calcd for $C_{83}H_{105}F_{24}N_9P_4Pt_3 \cdot CH_2Cl_2$ (found): C 39.70 (39.67), H 4.21 (4.38), N 4.96 (5.22).

[{Pt(^{t}Bu$_3$-trpy)}$_3$(μ$_3$-?^{1},?^{2}-C≡C-)](OTf)$_4$ (**1**·OTf) was prepared by the reaction of [Pt(^{t}Bu$_3$-trpy)(C≡C)Pt(^{t}Bu$_3$-trpy)](OTf)$_2$ with [Pt(^{t}Bu$_3$-trpy)(MeCN)](OTf)$_2$ in acetone. After stirring for 12 hours, a clear orange solution was obtained and the solvent was removed under vacuum. Subsequent recrystallization from slow vapor diffusion of *n*-hexane into a solution of **1**·OTf in dichloromethane yielded the pure form of **1**·OTf as yellowish-orange crystals. Yield: 85 %. ^{1}H NMR (500 MHz, CD_3COCD_3, 298 K, relative to Me_4Si): *d* = 1.34 (18H, *tert*-butyl H), 1.49 (s, 9H, *tert*-butyl H), 7.63 (dd, 2.0 and 6.0 Hz, 2H, 3- and 3'-protons on terpyridine), 8.74 (d, J = 2.0 Hz, 2H, 5- and 5"-protons on terpyridine), 8.80 (s, 2H, 3'-protons on terpyridine), 9.65 (d, J = 6.0 Hz, 2H, 2- and 2"-protons on terpyridine); ^{13}C{^{1}H} NMR (125.8 MHz, CD_3COCD_3, 298 K, relative to Me_4Si): *d* = 29.2 and 29.4 (primary C on *tert*-butyl group), 36.1 and 37.1 (quaternary C on *tert*-butyl group), 108.9 (C≡C), 121.8, 123.7, 126.5 and 154.0 (tertiary C on terpyridine), 154.6, 158.9, 167.4 and 168.6 (quaternary C on terpyridine); ^{195}Pt{^{1}H} NMR (107.2 MHz, CD_2Cl_2, 298 K, relative to Na_2PtCl_4 in D_2O): *d* = –2898; positive ESI-MS: m/z 2261 [*M*–OTf]$^+$, 1056 [*M*–2OTf]$^{2+}$; Raman: 1895 cm^{-1} ?(C≡C); elemental analysis (%) calcd for $C_{83}H_{105}F_{24}N_9P_4Pt_3 \cdot 2CH_2Cl_2$ (found): C 41.63 (41.64), H 4.36 (4.29), N 4.86 (4.82).

^{13}C enriched [{Pt(^{t}Bu$_3$-trpy)}$_3$(μ$_3$-?^{1},?^{2}-^{13}C≡^{13}C-)](OTf)$_4$ was prepared according to a procedure similar

to that of [{Pt(^{t}Bu$_3$-trpy)}$_3$(μ$_3$-?^{1},?^{2}-^{13}C≡^{13}C-)](OTf)$_4$ except ^{13}C enriched [Pt(^{t}Bu$_3$-trpy)(^{13}C≡^{13}C)Pt(^{t}Bu$_3$-trpy)](OTf)$_2$ was used. Yield: 85 %. ^{13}C{^{1}H} NMR (125.8 MHz, CD_3COCD_3, 298 K, relative to Me_4Si): *d* = 29.2 and 29.4 (primary C on *tert*-butyl group), 36.1 and 37.1 (quaternary C on *tert*-butyl group), 108.9 (C≡C, ^{195}Pt satellite signals with J_{C-Pt} = 574 Hz), 121.8, 123.7, 126.5 and 154.0 (tertiary C on terpyridine), 154.6, 158.9, 167.4 and 168.6 (quaternary C on terpyridine).

X-Ray Structure Determination

Crystal data for [{Pt(^{t}Bu$_3$-trpy)}$_3$(μ$_3$-?^{1},?^{2}-C≡C-)](PF$_6$)$_4$·(CH$_3$)$_2$CO: $C_{83}H_{105}F_{24}N_9P_4Pt_3$·$C_3H_6O$, *M*r = 2451.99, crystal dimensions 0.38 × 0.14 × 0.06 mm, triclinic, space group $P\bar{1}$, *a* = 17.926(5), *b* = 18.616(5), *c* = 19.583(4) Å, *a* = 65.881(7), *ß* = 77.724(6), *?* = 80.102(8) °, *V* = 5949(3) Å^3, *Z* = 2, ?$_{calcd}$ = 1.369 gcm^{-3}, *μ*(Mo$_{Ka}$) = 3.649 mm^{-1}, *F*(000) = 2416, *T* = 294 K. Final *R* = 0.0822, *wR*2 = 0.1504 with *I* > 2*s*(*I*); GOF = 0.987 for 1220 parameters and a total of 39406 reflections, of which 26778 were independent (R_{int} = 0.1938); Bruker CCD area diffractometer, Mo$_{Ka}$ radiation (? = 0.71073 Å); collection range 2*?* = 3.52 – 55.32°; phi and omega scan applied for diffraction measurement; 2416 frames taken in four shell.

Computational Details

Calculations were carried out using the Gaussian03 software package.[1] To reduce computational cost, model complexes [Pt(trpy)$_3$(μ$_3$-η^1,η^2-C=C-)]$^{4+}$ **1'** and [Pt(trpy)$_2$(C=C)Pt(trpy)]$^{2+}$ **2'** were used to mimic the complexes **1** and **2,** in which the *tert*-butyl groups at the 4-position of the pyridyl groups were replaced by hydrogen atoms. Geometry optimizations of **1'** (with C_2 symmetry), the transition state of the topomerization (with C_2 symmetry) and **2'** (with D_2 symmetry) were performed using density functional theory (DFT) at the hybrid Perdew, Burke, and Ernzerhof functional (PBE1PBE)[2] level of theory. Vibrational frequencies were calculated for all stationary points to verify that each was a minimum (NIMAG = 0) or a transition state (NIMAG = 1) on the potential energy surface. Based on the ground-

state optimized geometries in the gas phase, a nonequilibrium time-dependent (TDDFT) method at the same level was employed to study the nature of the low-lying singlet-singlet and singlet-triplet transitions. For all the calculations, the Stuttgart effective core potentials (ECPs) and the associated basis set were applied to describe Pt,[3] while the 6-31G basis set[4a,b] was used for all other atoms. Polarization functions have been added for the Pt atom (ζ_f(Pt)=0.997),[5] and the N and C atoms which are directly coordinated to the metal center [ζ_d(N) and ζ_d(C) = 0.8)].[4c]

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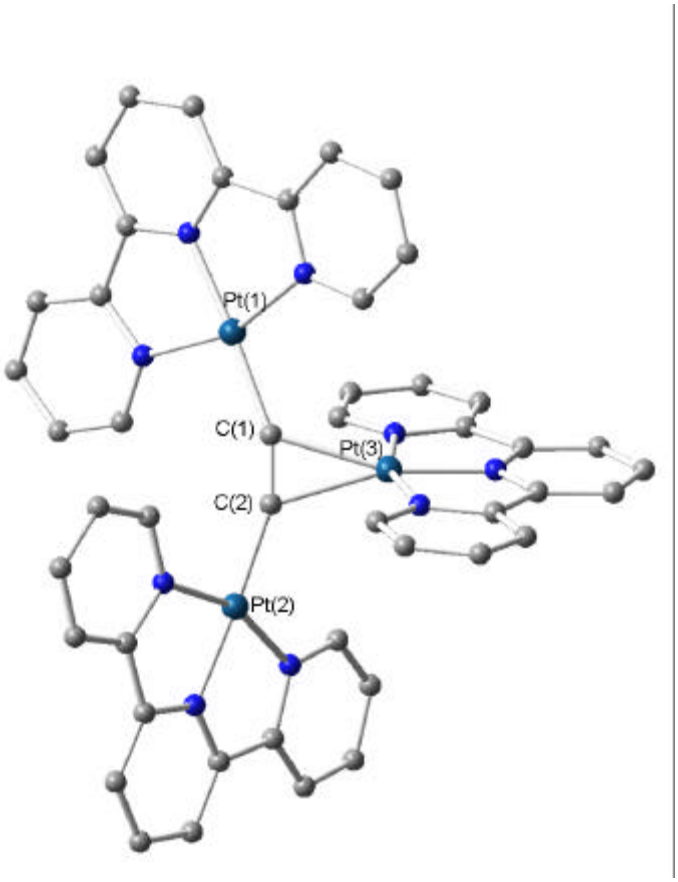

Figure S1 Optimized geometry of **1'**. Hydrogen atoms have been omitted for clarity.

Table S1 Selected structural parameters of the PBE1PBE optimized geometries in **1'** (with the experimental structural parameters of **1** in parentheses). Bond distances and angles are in Å and °, respectively. The atomic numbering is shown in Figure S1.

	1'
Pt(3)–C(1)	2.262 (2.198)
Pt(3)–C(2)	2.262 (2.198)
Pt(1)–C(1)	2.001 (1.953)
Pt(2)–C(2)	2.001 (2.043)
C(1)–C(2)	1.266 (1.249)
Pt–N[a]	2.022 (1.971)
Pt(1)–C(1)–C(2)	159.6 (154.6)
Pt(2)–C(2)–C(1)	159.6 (154.8)
Pt(3)–C(1)–C(2)	73.7 (73.5)
$\phi_{Pt(1)}$[b]	42.4 (43.5)
$\phi_{Pt(2)}$[b]	42.4 (43.2)
$\phi_{Pt(3)}$[b]	70.0 (68.2)

[a]Average Pt–N distance. [b]Interplanar angles between the triangular plane [Pt(3), C(1) and C(2) atoms] and [Pt(trpy)] plane.

Table S2 TDDFT vertical excitation wavelength (nm) of selected low-lying singlet (S_n) and the first triplet excited states (T_1) in **1'** and **2'** with the orbitals involved in the dominant excitation (H = HOMO and L = LUMO)

Complex	Transition	Dominant excitation	vertical excitation wavelength (nm)
1'	S_0 ? S_1 (0.016)[a]	H ? L (0.69)[b]	470
	S_0 ? T_1 (0.000)[a]	H ? L (0.68)[b]	490
2'	S_0 ? S_3 (0.317)[a]	H ? L (0.48)[b]	520
		H–1 ? L+1 (0.48)[b]	
	S_0 ? T_1 (0.000)[a]	H ? L (0.51)[b]	616
		H–1 ? L+1 (0.51)[b]	

[a]Oscillator strengths (*f*). [b]Transition coefficients.

Table S3 Cartesian coordinates for the PBE1PBE optimized structures of **1'**, the transition state for the topomerization, and **2'** with the calculated electronic energy (Hartree) in parenthesis.

1' (–2657.653077)

1	Pt	0.000000	0.000000	1.848861
2	C	0.150486	0.615062	-0.322429
3	C	-0.150486	-0.615062	-0.322429
4	Pt	0.762298	2.395200	-1.000140
5	Pt	-0.762298	-2.395200	-1.000140
6	N	1.403817	4.098346	-1.772117
7	C	2.272714	4.044772	-2.802810
8	C	0.957664	5.254089	-1.238909
9	C	2.753145	5.232139	-3.355660
10	C	1.409727	6.467922	-1.756933
11	C	2.314488	6.446428	-2.821384
12	H	3.451560	5.226110	-4.182648
13	H	1.073149	7.413642	-1.351845
14	H	2.677258	7.379109	-3.237495
15	N	1.973914	1.675257	-2.483105
16	C	2.591207	2.666446	-3.212406
17	C	2.196338	0.388726	-2.811522
18	C	3.442347	2.351957	-4.267477
19	C	3.037471	0.022953	-3.859570
20	H	1.677566	-0.350973	-2.214915
21	C	3.674279	1.016556	-4.599030
22	H	3.921337	3.141178	-4.833405
23	H	3.185148	-1.025368	-4.087536
24	H	4.335468	0.763712	-5.419704
25	N	-0.259236	3.726155	0.169847
26	C	-1.148367	3.452084	1.140466
27	C	0.000000	5.041848	-0.141015
28	C	-1.812900	4.449852	1.848883
29	H	-1.314318	2.402511	1.343821
30	C	-0.632888	6.076539	0.540889
31	C	-1.551538	5.784303	1.549261
32	H	-2.524765	4.180425	2.619023
33	H	-0.419117	7.106854	0.285444
34	H	-2.052325	6.584358	2.081834
35	N	-1.973914	-1.675257	-2.483105
36	C	-2.591207	-2.666446	-3.212406
37	C	-2.196338	-0.388726	-2.811522
38	C	-3.442347	-2.351957	-4.267477
39	C	-3.037471	-0.022953	-3.859570
40	H	-1.677566	0.350973	-2.214915
41	C	-3.674279	-1.016556	-4.599030
42	H	-3.921337	-3.141178	-4.833405
43	H	-3.185148	1.025368	-4.087536
44	H	-4.335468	-0.763712	-5.419704
45	N	-1.403817	-4.098346	-1.772117
46	C	-0.957664	-5.254089	-1.238909
47	C	-2.272714	-4.044772	-2.802810
48	C	-1.409727	-6.467922	-1.756933
49	C	-2.753145	-5.232139	-3.355660
50	C	-2.314488	-6.446428	-2.821384
51	H	-1.073149	-7.413642	-1.351845
52	H	-3.451560	-5.226110	-4.182648
53	H	-2.677258	-7.379109	-3.237495
54	N	0.259236	-3.726155	0.169847
55	C	1.148367	-3.452084	1.140466
56	C	0.000000	-5.041848	-0.141015
57	C	1.812900	-4.449852	1.848883
58	H	1.314318	-2.402511	1.343821
59	C	0.632888	-6.076539	0.540889
60	C	1.551538	-5.784303	1.549261
61	H	2.524765	-4.180425	2.619023
62	H	0.419117	-7.106854	0.285444
63	H	2.052325	-6.584358	2.081834
64	N	0.000000	0.000000	3.814692
65	C	1.181299	0.145544	4.453430
66	C	-1.181299	-0.145544	4.453430
67	C	1.204750	0.150753	5.848312
68	C	-1.204750	-0.150753	5.848312
69	C	0.000000	0.000000	6.540744
70	H	2.132087	0.267386	6.394642
71	H	-2.132087	-0.267386	6.394642
72	H	0.000000	0.000000	7.624722
73	N	-2.006310	-0.214281	2.191963
74	C	-2.991532	-0.299696	1.281362
75	C	-2.322957	-0.272015	3.530657
76	C	-4.328413	-0.451174	1.645146
77	H	-2.683190	-0.250060	0.245853
78	C	-3.641530	-0.428608	3.945573
79	C	-4.661053	-0.521090	2.995489
80	H	-5.089920	-0.513562	0.877756
81	H	-3.879460	-0.478249	5.000973
82	H	-5.691291	-0.642915	3.309484
83	N	2.006310	0.214281	2.191963
84	C	2.991532	0.299696	1.281362
85	C	2.322957	0.272015	3.530657
86	C	4.328413	0.451174	1.645146
87	H	2.683190	0.250060	0.245853
88	C	3.641530	0.428608	3.945573
89	C	4.661053	0.521090	2.995489
90	H	5.089920	0.513562	0.877756
91	H	3.879460	0.478249	5.000973
92	H	5.691291	0.642915	3.309484

The transition state for the topomerization (–2657.645301)

1	Pt	0.000000	0.000000	2.854224	75	C	-3.282210	-1.975891	-3.346369
2	C	0.000000	0.000000	0.911349	76	C	-2.274548	-3.834307	-2.264203
3	C	0.000000	0.000000	-0.361310	77	C	-4.084292	-2.823781	-4.111273
4	Pt	1.273849	1.282007	-1.417923	78	C	-3.054770	-4.721434	-3.006287
5	Pt	-1.273849	-1.282007	-1.417923	79	C	-3.962294	-4.203969	-3.934144
6	N	0.000000	0.000000	4.838277	80	H	-4.789939	-2.430228	-4.831667
7	C	1.159727	0.258493	5.476854	81	H	-2.966677	-5.792427	-2.875547
8	C	-1.159727	-0.258493	5.476854	82	H	-4.575786	-4.878146	-4.520441
9	C	1.184720	0.265821	6.871526	83	N	-0.630683	-3.079832	-0.673006
10	C	-1.184720	-0.265821	6.871526	84	C	0.295116	-3.298925	0.280314
11	C	0.000000	0.000000	7.563791	85	C	-1.267847	-4.160455	-1.241062
12	H	2.096351	0.470834	7.418022	86	C	0.635274	-4.579670	0.710096
13	H	-2.096351	-0.470834	7.418022	87	H	0.759030	-2.416533	0.701748
14	H	0.000000	0.000000	8.647637	88	C	-0.962659	-5.460024	-0.846840
15	N	-1.963527	-0.437035	3.211941	89	C	0.000000	-5.679659	0.139113
16	C	-2.931720	-0.639001	2.298948	90	H	1.386673	-4.704570	1.479964
17	C	-2.279017	-0.501882	4.550750	91	H	-1.472031	-6.300136	-1.302300
18	C	-4.247653	-0.912602	2.662424	92	H	0.243312	-6.688646	0.451313
19	H	-2.631015	-0.579179	1.259899					
20	C	-3.579585	-0.773361	4.963045					
21	C	-4.580350	-0.981128	4.012960					
22	H	-4.995180	-1.066267	1.894313					
23	H	-3.816635	-0.820621	6.018572					
24	H	-5.596493	-1.190069	4.326586					
25	N	1.963527	0.437035	3.211941					
26	C	2.931720	0.639001	2.298948					
27	C	2.279017	0.501882	4.550750					
28	C	4.247653	0.912602	2.662424					
29	H	2.631015	0.579179	1.259899					
30	C	3.579585	0.773361	4.963045					
31	C	4.580350	0.981128	4.012960					
32	H	4.995180	1.066267	1.894313					
33	H	3.816635	0.820621	6.018572					
34	H	5.596493	1.190069	4.326586					
35	N	2.414217	2.506225	-2.459959					
36	C	2.274548	3.834307	-2.264203					
37	C	3.282210	1.975891	-3.346369					
38	C	3.054770	4.721434	-3.006287					
39	C	4.084292	2.823781	-4.111273					
40	C	3.962294	4.203969	-3.934144					
41	H	2.966677	5.792427	-2.875547					
42	H	4.789939	2.430228	-4.831667					
43	H	4.575786	4.878146	-4.520441					
44	N	2.350179	-0.076506	-2.503325					
45	C	3.251829	0.504879	-3.365523					
46	C	2.276218	-1.418044	-2.452254					
47	C	4.071067	-0.272463	-4.178390					
48	C	3.077089	-2.241906	-3.239646					
49	H	1.546222	-1.824732	-1.767355					
50	C	3.988089	-1.664038	-4.119652					
51	H	4.773906	0.199679	-4.853400					
52	H	2.982965	-3.317695	-3.160098					
53	H	4.623570	-2.277642	-4.747497					
54	N	0.630683	3.079832	-0.673006					
55	C	-0.295116	3.298925	0.280314					
56	C	1.267847	4.160455	-1.241062					
57	C	-0.635274	4.579670	0.710096					
58	H	-0.759030	2.416533	0.701748					
59	C	0.962659	5.460024	-0.846840					
60	C	0.000000	5.679659	0.139113					
61	H	-1.386673	4.704570	1.479964					
62	H	1.472031	6.300136	-1.302300					
63	H	-0.243312	6.688646	0.451313					
64	N	-2.350179	0.076506	-2.503325					
65	C	-3.251829	-0.504879	-3.365523					
66	C	-2.276218	1.418044	-2.452254					
67	C	-4.071067	0.272463	-4.178390					
68	C	-3.077089	2.241906	-3.239646					
69	H	-1.546222	1.824732	-1.767355					
70	C	-3.988089	1.664038	-4.119652					
71	H	-4.773906	-0.199679	-4.853400					
72	H	-2.982965	3.317695	-3.160098					
73	H	-4.623570	2.277642	-4.747497					
74	N	-2.414217	-2.506225	-2.459959					

2' (–1797.456632)

1	C	0.000000	0.000000	7.268156
2	C	0.000000	1.215025	6.577834
3	C	0.000000	1.190124	5.183113
4	N	0.000000	0.000000	4.548566
5	C	0.000000	-1.190124	5.183113
6	C	0.000000	-1.215025	6.577834
7	Pt	0.000000	0.000000	2.578221
8	N	0.000000	1.994824	2.911260
9	C	0.000000	2.330526	4.246039
10	C	0.000000	3.664985	4.638475
11	C	0.000000	4.670476	3.671299
12	C	0.000000	4.313573	2.325523
13	C	0.000000	2.964207	1.980561
14	C	0.000000	-2.330526	4.246039
15	N	0.000000	-1.994824	2.911260
16	C	0.000000	-2.964207	1.980561
17	C	0.000000	-4.313573	2.325523
18	C	0.000000	-4.670476	3.671299
19	C	0.000000	-3.664985	4.638475
20	Pt	0.000000	0.000000	-2.578221
21	N	-1.994824	0.000000	-2.911260
22	C	-2.330526	0.000000	-4.246039
23	C	-3.664985	0.000000	-4.638475
24	C	-4.670476	0.000000	-3.671299
25	C	-4.313573	0.000000	-2.325523
26	C	-2.964207	0.000000	-1.980561
27	C	-1.190124	0.000000	-5.183113
28	N	0.000000	0.000000	-4.548566
29	C	1.190124	0.000000	-5.183113
30	C	1.215025	0.000000	-6.577834
31	C	0.000000	0.000000	-7.268156
32	C	-1.215025	0.000000	-6.577834
33	C	2.330526	0.000000	-4.246039
34	N	1.994824	0.000000	-2.911260
35	C	2.964207	0.000000	-1.980561
36	C	4.313573	0.000000	-2.325523
37	C	4.670476	0.000000	-3.671299
38	C	3.664985	0.000000	-4.638475
39	H	2.621427	0.000000	-0.952712
40	H	5.064436	0.000000	-1.545676
41	H	5.712460	0.000000	-3.968280
42	H	3.921487	0.000000	-5.690497
43	H	2.149988	0.000000	-7.123342
44	H	0.000000	0.000000	-8.351520
45	H	-2.149988	0.000000	-7.123342
46	H	-3.921487	0.000000	-5.690497
47	H	-5.712460	0.000000	-3.968280
48	H	-5.064436	0.000000	-1.545676
49	H	0.000000	2.621427	0.952712
50	H	0.000000	5.064436	1.545676
51	H	0.000000	5.712460	3.968280
52	H	0.000000	3.921487	5.690497
53	H	0.000000	-2.621427	0.952712
54	H	0.000000	-5.064436	1.545676
55	H	0.000000	-5.712460	3.968280
56	H	0.000000	-3.921487	5.690497
57	H	0.000000	2.149988	7.123342
58	H	0.000000	0.000000	8.351520
59	H	0.000000	-2.149988	7.123342
60	H	-2.621427	0.000000	-0.952712
61	C	0.000000	0.000000	-0.619310
62	C	0.000000	0.000000	0.619310