

Supplementary information

Luminescence of Tartrate Bridged Dinuclear 2,2'-Bipyridine Platinum(II) Complexes: Emission Color Controlled by Intra- and Inter-molecular Interactions in the Solid State

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Table S1. Summary of crystallographic data for crystals of **1 α** , **1 β** , **2·12.5H₂O**, **3·4H₂O**, and **4·H₂O**.

	1α	1β	2·12.5H₂O
CCDC deposition number	1502815	1502814	1502817
formula	C ₂₄ H ₃₀ N ₄ O ₁₂ Pt ₂	C ₂₄ H ₃₀ N ₄ O ₁₂ Pt ₂	C ₄₈ H ₈₆ N ₈ O ₃₇ Pt ₄
formula weight	956.70	956.70	2147.60
temperature (K)	200	200	200
crystal system	Monoclinic	Triclinic	Monoclinic
space group	<i>P</i> 2(1)	<i>P</i> 1	<i>C</i> 2/ <i>c</i>
<i>a</i> [Å]	10.6927(8)	7.2798(5)	23.328(6)
<i>b</i> [Å]	18.9465(14)	10.3151(7)	15.799(4)
<i>c</i> [Å]	21.1599(16)	20.0355(14)	22.403(6)
α [deg]	90.00	102.1730(10)	90.00
β [deg]	92.9650(10)	93.9140(10)	120.006(3)
γ [deg]	90.00	100.8320(10)	90.00
<i>V</i> [Å ³]	4281.0(6)	1435.32(17)	7150(3)
Flack parameter	-0.005(4)	0.013(4)	-
<i>Z</i>	6	2	4
ρ (cal) (g/cm ³)	2.212	2.214	1.995
μ (mm ⁻¹)	9.862	9.805	7.897
<i>F</i> (000)	2724	908	4152
Reflections collected	44724	14758	35844
Independent reflections	16712 [<i>R</i> (int) = 0.0352]	10848 [<i>R</i> (int) = 0.0180]	7030 [<i>R</i> (int) = 0.0709]
<i>R</i> ₁ [<i>I</i> > 2 σ (<i>I</i>)]	0.0247	0.0170	0.0549
<i>wR</i> ₂ (all)	0.0520	0.0397	0.1439
<i>GOF</i>	0.934	0.761	1.129

	3·4H₂O	4·H₂O
CCDC deposition number	1502816	1502818
formula	C ₂₄ H ₂₆ N ₄ O ₁₀ Pt ₂	C ₁₄ H ₁₄ N ₂ O ₇ Pt
formula weight	920.67	517.36
temperature (K)	200	200
crystal system	Monoclinic	Monoclinic
space group	<i>P</i> 2(1)/ <i>n</i>	<i>Cc</i>
<i>a</i> [Å]	11.4751(8)	7.6436(9)
<i>b</i> [Å]	19.2533(14)	22.957(3)
<i>c</i> [Å]	11.9630(8)	8.8476(11)
α [deg]	90.00	90.00
β [deg]	104.5810(10)	102.6920(10)
γ [deg]	90.00	90.00
<i>V</i> [Å ³]	2557.9(3)	1514.6(3)
Flack parameter	-	-
<i>Z</i>	4	4
ρ (cal) (g/cm ³)	2.391	2.269
μ (mm ⁻¹)	10.993	9.306
<i>F</i> (000)	1736	984
Reflections collected	27798	7969
Independent reflections	5434 [<i>R</i> (int) = 0.0253]	3098 [<i>R</i> (int) = 0.0219]
<i>R</i> ₁ [<i>I</i> > 2σ(<i>I</i>)]	0.0185	0.0131
<i>wR</i> ₂ (all)	0.0425	0.0302
<i>GOF</i>	1.039	0.850

Table S2. Selected bond lengths (Å) for **1 α** , **1 β** , **2**·12.5H₂O, **3**·4H₂O, and **4**·H₂O.

	1α	1β	2 ·12.5H ₂ O	3 ·4H ₂ O	4 ·H ₂ O
C1–O1	1.306(13)	1.299(8)	1.291(16)	1.309(5)	1.291(6)
C1–O2	1.238(12)	1.230(9)	1.225(17)	1.223(5)	1.231(6)
C2–O3	1.410(11)	1.409(9)	1.440(14)	1.405(4)	1.402(10)
C3–O4	1.399(12)	1.404(8)	1.379(16)	1.421(5)	1.407(8)
C4–O5	1.310(12)	1.306(10)	1.305(17)	1.300(5)	1.322(6)
C4–O6	1.232(12)	1.230(8)	1.249(17)	1.222(5)	1.190(6)

Table S3. Hydrogen bonding parameters between complexes and between complex and lattice water molecules in **1 α** , **1 β** , and **4·H₂O**.

complex	<i>D</i> –H... <i>A</i>	<i>D</i> –H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>DHA</i>
1α	O1S–H1SB...O10	0.87	1.84	2.674(9)	160.9
	O2S–H2SA...O4	0.87	1.75	2.622(10)	179.5
	O2S–H2SB...O9	0.87	1.84	2.668(10)	159.3
	O5S–H5SA...O16	0.87	1.97	2.694(9)	139.3
	O5S–H5SB...O3 ^{<i>i</i>}	0.87	1.86	2.670(10)	153.2
1β	O1S–H1SA...O3	0.87	1.89	2.724(8)	160.4
	O6S–H6SA...O1 ^{<i>i</i>}	0.87	2.11	2.915(8)	154.3
	O6S–H6SB...O4 ^{<i>ii</i>}	0.87	1.92	2.696(8)	147.2
	O7S–H7SA...O7 ^{<i>iii</i>}	0.87	1.93	2.797(7)	179.6
	O7S–H7SB...O10	0.87	1.81	2.666(7)	168.1
	O10S–H10B...O9 ^{<i>iii</i>}	0.87	1.79	2.662(7)	179.8
4·H₂O	O1S–H1O...O6 ^{<i>v</i>}	0.824(15)	2.02(2)	2.817(8)	163(7)
	O1S–H2O...O3	0.828(15)	1.88(2)	2.707(10)	174(9)
	C3–H3...O6 ^{<i>iv</i>}	1.00	2.62	3.579(8)	161.0
	O4–H4...O1S ^{<i>iii</i>}	0.84	1.85	2.679(8)	171.4
	O5–H5A...O2 ^{<i>vi</i>}	0.84	1.84	2.650(5)	161.5

i: *x*, *y*+1, *z*; *ii*: *x*+1, *y*+1, *z*; *iii*: *x*–1, *y*, *z*; *iv*: –0.5+*x*, 1.5–*y*, –0.5+*z*; *v*: *x*+0.5, –*y*+1.5, *z*–0.5; *vi*: *x*+0.5, –*y*+1.5, *z*+0.5.