

Supporting Information

Ultrasound-Induced Emission Enhancement Based on Structure-Dependent Homo- and Heterochiral Aggregations of Chiral Binuclear Platinum Complexes

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Table S1. Crystallographic data for (\pm)-*anti*-**1a**, (+)-*anti*-**1a**, (\pm)-*anti*-**1c** and (+)-*anti*-**1c**.

	(\pm)- <i>anti</i> - 1a	(+)- <i>anti</i> - 1a •C ₆ H ₁₂	(\pm)- <i>anti</i> - 1c	(+)- <i>anti</i> - 1c •2.5C ₆ H ₁₂
Formula	C ₃₈ H ₄₀ N ₄ O ₄ Pt ₂	C ₃₈ H ₄₀ N ₄ O ₄ Pt ₂ •C ₆ H ₁₂	C ₄₂ H ₄₈ N ₄ O ₄ Pt ₂	C ₄₂ H ₄₈ N ₄ O ₄ Pt ₂ •2.5C ₆ H ₁₂
Formula weight	1006.94	1091.10	1063.05	1273.45
Temperature (K)	114	114	113	113
Crystal color, habit	orange, platelet	orange, block	orange, block	orange, needle
Crystal size, mm	0.80×0.80×0.10	0.10×0.05×0.05	0.20×0.20×0.10	0.40×0.05×0.05
Crystal system	monoclinic	monoclinic	monoclinic	orthorhombic
Space group	P2/n (#13)	C2 (#5)	P2 ₁ /c (#14)	P2 ₁ 2 ₁ 2 (#18)
<i>a</i> , Å	16.539(6)	38.64(3)	9.796(3)	18.1342(3)
<i>b</i> , Å	9.781(3)	9.835(6)	19.219(5)	21.0565(3)
<i>c</i> , Å	22.109(8)	10.795(7)	20.060(6)	14.0388(2)
α , deg	90	90	90	90
β , deg	108.690(5)	94.461(12)	99.104(8)	90
γ , deg	90	90	90	90
<i>V</i> , Å ³	3388(2)	4090(5)	3729.0(17)	5360.6(2)
Z value	4	4	4	4
<i>D</i> _{calcd} , gcm ⁻³	1.974	1.772	1.893	1.578
μ (MoK α), cm ⁻¹	82.632	68.526	75.131	52.407
<i>F</i> (000)	1936.00	2128.00	2064.00	2544.00
2 θ _{max} , deg	55.0	54.9	55.0	54.9
No. of reflns measd	24510	19102	47624	107204
No. obsd reflns	7707	9017	8515	12197
No. variables	433	363	470	604
<i>R</i> ₁ (I > 2 σ (I))	0.078	0.10	0.078	0.031
w <i>R</i> ₂ (all reflns)	0.22	0.24	0.25	0.062
goodness of fit	1.09	1.04	1.22	1.07
Flack parameter		0.01(3)		0.002(6)

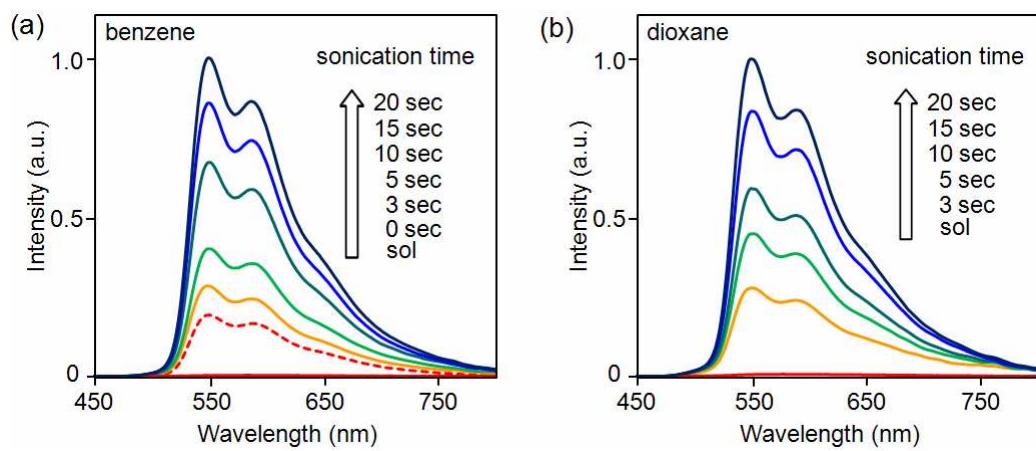


Figure S1. Emission spectra of gels of (\pm) -anti-**1a** in (a) benzene (1.20×10^{-2} M) and (b) 1,4-dioxane (2.00×10^{-2} M) generated by sonication (44 kHz, 0.31 W/cm 2) for various irradiation times ($\lambda_{\text{ex}} = 420$ nm, 293 K). Dashed line: a spontaneous gel formed by standing at room temperature for 1 h without sonication.

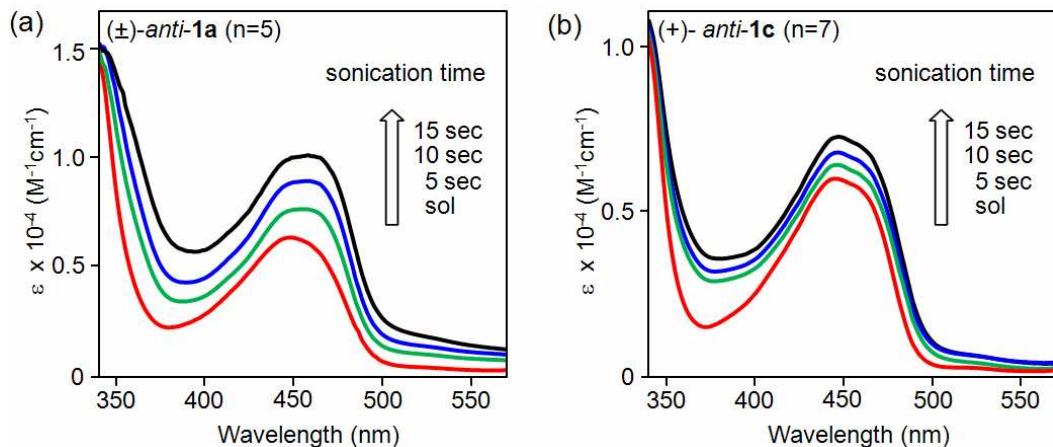


Figure S2. UV-vis spectra of (a) (\pm) -anti-**1a** and (b) $(+)$ -anti-**1c** gels in cyclohexane (1.50×10^{-3} M) generated by sonication (44 kHz, 0.31 W/cm 2) for various times.

Table S2. Excitation energy, oscillator strength and major electronic configuration of *anti-1a*.^a

state	excitation energy (eV)	oscillator strength	major configuration ^b	coefficient
Singlet state				
1	2.6321	f = 0.0224	182→183	0.61052
2	2.7426	0.0283	181→184	-0.44011
			182→184	0.49642
3	2.8775	0.0001	181→183	0.55377
4	2.8893	0.0019	182→185	0.41429
Triplet state				
1	2.1618		182→183	0.52554
2	2.2820		181→184	0.49384
			182→184	-0.40389
3	2.3934		182→185	0.49460
4	2.5085		181→186	-0.37756
			182→186	0.38037

^a Estimated by TD-DFT (B3LYP/6-31G*, LanL2DZ) calculations based on the X-ray structure of (\pm)-**anti-1a**. ^b HOMO is MO182.

Table S3. Excitation energy, oscillator strength and major electronic configuration of *anti-1c*.^a

state	excitation energy (eV)	oscillator strength	major configuration ^b	coefficient
Singlet state				
1	2.6742	f = 0.0250	198→199	0.63808
2	2.7402	0.0357	197→200	0.61234
3	2.9638	0.0009	197→199	0.60422
4	2.9657	0.0006	198→200	0.57951
Triplet state				
1	2.2039		198→199	0.60527
2	2.2750		197→200	0.59301
3	2.4803		198→201	0.48859
4	2.5056		197→202	0.46855

^a Estimated by TD-DFT (B3LYP/6-31G*, LanL2DZ) calculations based on the X-ray structure of (+)-**anti-1c**. ^b HOMO is MO198.

Complete reference 20.

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