# **Supporting Information**

# Solution-state Mechanochromic Luminescence of Pt(II)complexes Displayed within Micellar Aromatic Capsules

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## Contents

- Materials and methods, and References
- Synthesis of **PBA** (<sup>1</sup>H, <sup>13</sup>C NMR and MS spectra)
- Formation of capsule (**PBA**)<sub>*n*</sub> (<sup>1</sup>H, <sup>13</sup>C, DOSY NMR spectra, DLS charts, UV-visible, fluorescence spectra, and optimized structure)
- Synthesis of Pt-complex 2 (<sup>1</sup>H NMR spectra)
- Synthesis of Pt-complex **1a** (<sup>1</sup>H NMR and MS spectra)
- Synthesis of Pt-complexes **1b** and **1c** (<sup>1</sup>H, <sup>13</sup>C, DEPT 90 NMR and MS spectra)
- Crystal structure and data of **1c**
- Formation of (PBA)<sub>n</sub>•(1a)<sub>m</sub> via grinding (<sup>1</sup>H, DLS, UV-visible, and emission data, and optimized structure)
- Formation of (**PBA**)<sub>*n*</sub>•(**1a**)<sub>*m*</sub>•(**BC**)<sub>*p*</sub> (<sup>1</sup>H, DLS, AFM, UV-visible, and emission data)
- Formation of  $(\mathbf{PBA})_n \bullet (\mathbf{1a})_m$  via stirring (UV-visible and emission spectra)
- Solid-state properties of **1a-c** (emission spectra)

### Materials and methods

NMR: Bruker AVANCE-400 (400 MHz) and AVANCE III HD 500 (500 MHz), GC MS: Shimadzu Parvum2/ULBON HR-1, ESI-TOF MS: Bruker micrOTOF II, UV-visible: JASCO V-670DS, Fluorescence: Hitachi F-7000, Absolute PL quantum yield: Hamamatsu C9920-02G with an integration sphere, Fluorescence lifetime: Hamamatsu C7700-ABS-N, FT-IR: SHIMADZU IRSpirit-T, DLS: Wyatt Technology DynaPro NanoStar, AFM: Asylum Research Cypher S, XRD: Rigaku XtaLAB Synergy-DW.

Molecular mechanics calculation (geometry optimization): Forcite module, BIOVIA Materials Studio 2020, version 20.1.0.5 (Dassault Systèmes Co.).

Solvents and reagents were purchased from TCI Co., Ltd., FUJIFILM Wako Chemical Co., Kanto Chemical Co., Inc., Sigma-Aldrich Co., and Cambridge Isotope Laboratories, Inc. Compound **PB-OH** was synthesized according to ref. S6.

### References

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**PB-OH**<sup>[S1]</sup> (188 mg, 0.466 mmol), NaOH (932 mg, 23.3 mmol), and dry toluene (10 mL) were added to a 20 mL Pyrex pressure vessel. The mixture was stirred at 80 °C for 30 min. 2-Chloro-N,N-dimethylethanamine hydrochloride (540 mg, 3.75 mmol) was added to the reaction mixture at r.t. The resultant mixture was stirred at 130 °C overnight. The resultant mixture was filtered at r.t., and then concentrated under reduced pressure. The crude product was extracted with EtOAc ( $3 \times 20$  mL). The combined organic phase was dried over MgSO<sub>4</sub>, filtrated, and concentrated under reduced pressure to afford PB-NMe<sub>2</sub> (242 mg, 0.444 mmol, 95%) as a white solid.<sup>[S2]</sup> PB-NMe<sub>2</sub> (242 mg, 0.444 mmol), CH<sub>3</sub>I (0.60 mL, 9.70 mmol), and dry CH<sub>3</sub>CN (4.0 mL) were added to a 2-necked 50 mL glass flask. The mixture was stirred at r.t. overnight. The precipitate was collected by filtration to afford **PB-NMe<sub>3</sub>** (250 mg, 0.302 mmol, 68%) as a white solid.<sup>[S2]</sup> **PB-NMe<sub>3</sub>** (257 mg, 0.309 mmol), AgCl (220 mg, 1.54 mmol), and H<sub>2</sub>O (4.0 mL) were added to a 2-necked 10 mL glass flask. The mixture was stirred at 80 °C overnight. After the addition of CH<sub>3</sub>OH (10 mL), the resultant solution was centrifugated, filtered, and concentrated under reduced pressure. The crude product was washed with acetone, CHCl<sub>3</sub> to afford **PBA** (177 mg, 0.274 mmol, 89%) as a white solid.<sup>[S2]</sup>

**PBA**: <sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD, r.t.):  $\delta$  2.00 (s, 12H), 2.23 (s, 12H), 2.27 (s, 6H), 2.86 (s, 18H), 3.64 (t, *J* = 4.6 Hz, 4H), 4.44 (br, 4H), 6.69 (s, 1H), 7.06 (s, 1H). <sup>13</sup>C NMR (100 MHz, CD<sub>3</sub>OD, r.t.):  $\delta$  15.3 (CH<sub>3</sub>), 17.0 (CH<sub>3</sub>), 53.1 (CH<sub>3</sub>), 63.3 (CH<sub>2</sub>), 64.8 (CH<sub>2</sub>), 100.3 (CH), 126.5 (C<sub>q</sub>), 131.5 (C<sub>q</sub>), 132.1 (C<sub>q</sub>), 132.7 (CH), 133.8 (C<sub>q</sub>), 134.9 (C<sub>q</sub>), 154.5 (C<sub>q</sub>). FT-IR (ATR, cm<sup>-1</sup>): 3370, 3006, 2920, 1605, 1580, 1475, 1418, 1324, 1276, 1247, 1187, 1164, 1111, 1066, 958, 882, 792, 646. ESI-TOF MS (CH<sub>3</sub>OH): *m*/*z* 609.5 [M – Cl<sup>-</sup>]<sup>+</sup>, 287.3 [M – 2•Cl<sup>-</sup>]<sup>2+</sup>.







Figure S3. ESI-TOF MS spectrum (CH<sub>3</sub>OH) of PBA.



Amphiphile **PBA** (1.3 mg, 2.0  $\mu$ mol) was added to water (2.0 mL) and the solution was stirred at r.t. for 1 min to give a clear solution including capsule (**PBA**)<sub>n</sub>. The quantitative formation and structure of (**PBA**)<sub>n</sub> were confirmed by <sup>1</sup>H and <sup>13</sup>C NMR, DOSY NMR, and DLS analyses. The optimized structure of capsule (**PBA**)<sub>4</sub> was obtained by molecular mechanics calculation (Forcite module, Materials Studio).

<sup>1</sup>H NMR (400 MHz, D<sub>2</sub>O, r.t., 40 mM based on **PBA**):  $\delta$  1.69 (s, 12H), 1.90 (s, 12H), 1.99 (s, 6H), 2.67 (s, 18H), 3.46 (s, 4H), 4.24 (s, 4H), 6.33 (s, 1H), 6.85 (s, 1H). <sup>13</sup>C NMR (100 MHz, D<sub>2</sub>O, r.t., 40 mM based on **PBA**):  $\delta$  15.7 (CH<sub>3</sub>), 15.8 (CH<sub>3</sub>), 17.3 (CH<sub>3</sub>), 53.6 (CH<sub>3</sub>), 63.5 (CH<sub>2</sub>), 65.0 (CH<sub>2</sub>), 101.2 (CH), 126.8 (C<sub>q</sub>), 131.7 (C<sub>q</sub>), 132.3 (C<sub>q</sub>), 132.6 (CH), 134.5 (C<sub>q</sub>), 134.6 (C<sub>q</sub>), 154.3 (C<sub>q</sub>). DOSY NMR (500 MHz, D<sub>2</sub>O, 40 mM based on **PBA**, 25 °C):  $D = 3.08 \times 10^{-10} \text{ m}^2 \text{ s}^{-1}$ .



Figure S4b. <sup>1</sup>H NMR spectrum (400 MHz,  $D_2O$ , r.t., 40 mM based on PBA) of (PBA)<sub>n</sub>.





D20

6 9137 MHz EM

0.30 Hz 0 1.00

QF 500.1363894 MHz no 0 0 Hz 0

F2 - Pr SI SF WDW SSB LB GB PC

F1 - P SI MC2 SF WDW SSB LB GB

-8.4

-8.2

ppm

500

Figure S6. DOSY NMR spectrum (500 MHz, D<sub>2</sub>O, 40 mM based on PBA, 298 K) of (PBA)<sub>n</sub>.

2

1

0

3

7

6

10

9

8

5

4



Figure S7. UV-visible spectra (r.t., 2.0 mM based on PBA) of  $(PBA)_n$  in H<sub>2</sub>O and PBA in CH<sub>3</sub>OH.



**Figure S8.** Concentration-dependent fluorescence spectra (r.t., 0.001-1.0 mM based on **PBA**,  $\lambda_{ex} = 284$  nm) of (**PBA**)<sub>n</sub> in H<sub>2</sub>O.



Figure S9. a) DLS chart (H<sub>2</sub>O, r.t., 2.0 mM based on PBA) of capsule (PBA)<sub>n</sub> and b) the optimized structure of (PBA)<sub>4</sub>.



2-Bromopyridine (3.00 mL, 30.9 mmol) and dry THF (80 mL) were added to a 2necked 300 mL glass flask filled with N<sub>2</sub>. After stirring at -80 °C for 30 min, a hexane solution (2.69 M) of *n*-butyllithium (13.0 mL, 35.0 mmol) was added dropwise to the 300 mL flask at -80 °C under N<sub>2</sub>. After stirring the mixture at -80 °C for 1 h, a dry THF solution (20 mL) of ZnCl<sub>2</sub> (5.80 g, 41.9 mmol) was added to the solution. The resultant mixture was further stirred at -80 °C for 1 h, and then the solution was warmed to r.t. for 30 min to obtain 2-pyridylzinc chloride. 1,3-Dibromobeneze (1.30 mL, 10.8 mmol),  $Pd(PPh_3)_4$  (0.580 g, 0.502 mmol), and dry THF (40 mL) were added to a 50 mL glass flask filled with N<sub>2</sub>. After stirring the mixture for 30 min at r.t., the mixture was added to the 300 mL flask, and then the resulted solution was further stirred at 80 °C overnight. After the addition of CH<sub>3</sub>OH (50 mL) at 0 °C, the reaction mixture was filtered through a short pad of Celite and then concentrated under reduced pressure. The crude product was extracted with  $CH_2Cl_2$  (3 × 20 mL). The combined organic phase was washed with H<sub>2</sub>O (30 mL) and brine (30 mL), dried over MgSO<sub>4</sub>, filtrated, and concentrated under reduced pressure. The crude product was purified by column chromatography (hexane/ethyl acetate = 2:1) to afford 1,3-di(2-pyridyl)benzene (1.70 g, 7.32 mmol, 73%) as yellow liquid.<sup>[S3]</sup>

1,3-Di(2-pyridyl)benzene (116 mg, 0.500 mmol),  $K_2PtCl_4$  (174 mg, 0.420 mmol), and 9:1 acetic acid/H<sub>2</sub>O solution (1.5 mL) were added to a 2.0 mL Pyrex pressure vessel. The mixture was heated at 160 °C for 3 h by a microwave reactor (2450 MHz). After the filtration of the suspended reaction mixture at r.t., the obtained solid was washed with H<sub>2</sub>O, CH<sub>3</sub>OH, and diethyl ether, and dried under vacuum to afford Pt-complex **2** (153 mg, 0.331 mmol, 66%) as an orange solid.<sup>[54]</sup>

1,3-Di(2-pyridyl)benzene: <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, r.t.):  $\delta$  7.40 (ddd, J = 7.8, 4.8, 0.91 Hz, 2H), 7.63 (t, J = 7.8 Hz, 1H), 7.93 (td, J = 7.8, 1.8 Hz, 2H), 8.09 (dt, J = 7.8, 0.91 Hz, 2H), 8.16 (dd, J = 7.8, 1.8 Hz, 2H), 8.72 (ddd, J = 4.8, 1.8, 0.84 Hz, 2H), 8.82 (t, J = 1.8 Hz, 1H). GC MS: m/z Calcd. for C<sub>16</sub>H<sub>12</sub>N<sub>2</sub> 232 [M]<sup>+</sup>, Found 232.

Pt-complex **2**: <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, r.t.):  $\delta$  7.30 (t, J = 7.7 Hz, 1H), 7.54-7.58 (m, 2H), 7.78 (d, J = 7.7 Hz, 2H), 8.14 (d, J = 7.6 Hz, 2H), 8.21 (td, J = 7.6, 1.6 Hz, 2H), 9.07-9.17 (m, 2H). ESI-TOF MS: m/z Calcd. For C<sub>16</sub>H<sub>11</sub>N<sub>2</sub>ClPt 426.1 [M – Cl]<sup>+</sup>, Found 426.1.



Figure S10. <sup>1</sup>H NMR spectrum (400 MHz, DMSO-*d*<sub>6</sub>, r.t.) of 1,3-di(2-pyridyl)benzene.



**Figure S11.** <sup>1</sup>H NMR spectrum (400 MHz, DMSO-*d*<sub>6</sub>, r.t.) of Pt-complex **2**.



A mixture of phenylacetylene (0.10 mL, 0.91 mmol), NaOH (18.0 mg, 0.450 mmol), and CH<sub>3</sub>OH (2.0 mL) was stirred at r.t. for 1 h in a screw-cap test tube. Pt-complex **2** (90.0 mg, 0.194 mmol) was added to the test tube and the reaction mixture was stirred overnight. After filtration at r.t., the obtained solid was washed with H<sub>2</sub>O, CH<sub>3</sub>OH, and hexane, and dried under vacuum to afford Pt-complex **1a** (85.9 mg, 0.163 mmol, 86%) as a yellow solid.<sup>[85]</sup>

Pt-complex **1a**: <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, r.t.):  $\delta$ 7.17-7.23 (m, 4H), 7.29 (t, *J* = 7.3 Hz, 2H), 7.52 (d, *J* = 7.7 Hz, 2H), 7.58-7.60 (m, 2H), 7.68 (d, *J* = 7.6 Hz, 2H), 7.92 (td, *J* = 7.6, 1.6 Hz, 2H), 9.45-9.58 (m, 2H). ESI-TOF MS (CH<sub>2</sub>Cl<sub>2</sub>): *m/z* Calcd. For C<sub>24</sub>H<sub>16</sub>N<sub>2</sub>Pt 526.2 [M – H]<sup>+</sup>, Found 526.1.







Figure S13. ESI-TOF MS spectrum (CH<sub>2</sub>Cl<sub>2</sub>) of Pt-complex 1a.

Synthesis of Pt-complexes 1b and 1c YH070-072, 074, 076, 078  $\begin{array}{c} \downarrow & \downarrow & \downarrow \\ - si & = & \downarrow \\$ 

1-Iodo-4-methoxybenzene (1.00 g, 4.27 mmol),  $Pd(PPh_3)_2Cl_2$  (120 mg, 0.171 mmol), CuI (16.3 mg, 0.100 mmol), and dry THF (10 mL) were added to a 2-necked 50 mL glass flask filled with N<sub>2</sub>. Trimethysilylacetylene (1.20 mL, 8.66 mmol) and Et<sub>3</sub>N (10 mL) were added to a 2-necked 25 mL glass flask. After being degassed by sonication under N<sub>2</sub>, the mixture was added to the 50 mL glass flask and then stirred at r.t. overnight. The reaction mixture was filtered through a silica gel and then concentrated under reduced pressure. The crude product was purified by column chromatography (hexane) to afford ((4-methoxyphenyl)ethynyl)trimethylsilane (784 mg, 3.84 mmol, 90%) as colorless liquid.<sup>[S6]</sup>

((4-Methoxyphenyl)ethynyl)trimethylsilane (326 mg, 1.60 mmol), K<sub>2</sub>CO<sub>3</sub> (663 mg, 4.79 mmol), dry THF (7.0 mL), and CH<sub>3</sub>OH (3.0 mL) were added to a 2-necked 50 mL glass flask. The mixture was stirred at r.t. for 3 h. The reaction mixture was filtered through a silica gel and then concentrated under reduced pressure. The crude product was extracted with CH<sub>2</sub>Cl<sub>2</sub> ( $3 \times 20$  mL). The combined organic phase was dried over MgSO<sub>4</sub>, filtrated, and concentrated under reduced pressure to afford 1-ethynyl-4-methoxybenzene (175 mg, 1.32 mmol, 83%) as yellow liquid.<sup>[S6]</sup> A mixture of 1-ethynyl-4-methoxybenzene (22.0 mg, 0.167 mmol), NaOH (10.0 mg, 0.250 mmol), and CH<sub>3</sub>OH (2.0 mL) was stirred at r.t. for 1.5 h in a 2-necked 10 mL glass flask. Pt-complex **2** (50.2 mg, 0.109 mmol) was added to the 10 mL glass flask and the reaction mixture was stirred overnight. After filtration at r.t., the obtained solid was washed with H<sub>2</sub>O, CH<sub>3</sub>OH, and hexane, and dried under vacuum to afford Pt-complex **1b** (43.4 mg, 77.8 µmol, 72%) as an orange solid.<sup>[85]</sup>

The same procedure using Pt-complex **2** (30.5 mg, 66.0 mmol) and 1-ethynyl-4-(trifluoromethyl)benzene (23.9 mg, 0.140 mmol) afforded Pt-complex **1c** (21.8 mg, 36.6 mmol, 56%) as a yellow solid.<sup>[S7]</sup> Pt-complex **1b**: <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, r.t.):  $\delta$  3.82 (s, 3H), 6.84 (d, *J* = 8.8 Hz, 2H), 7.18-7.23 (m, 3H), 7.52 (dd, *J* = 8.8, 3.2 Hz, 4H), 7.67 (d, *J* = 7.8 Hz, 2H), 7.92 (td, *J* = 7.8, 1.6 Hz, 2H), 9.47-9.60 (m, 2H). <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>, r.t.):  $\delta$  55.5 (CH<sub>3</sub>), 110.9 (C<sub>q</sub>), 114.2, 120.8, 121.5 (C<sub>q</sub>), 123.6, 124.9×2, 132.6, 136.7 (C<sub>q</sub>), 140.3, 143.2 (C<sub>q</sub>), 155.0, 157.4 (C<sub>q</sub>), 169.3 (C<sub>q</sub>), 178.3 (C<sub>q</sub>). FT-IR (ATR, cm<sup>-1</sup>): 3062, 3007, 2951, 2902, 2834, 2082, 1597, 1500, 1483, 1464, 1391, 1321, 1293, 1277, 1239, 1208, 1163, 1100, 1027, 844, 814, 783, 762, 749, 742, 722, 634, 544, 501, 482, 449. HR-MS (CH<sub>2</sub>Cl<sub>2</sub>): *m/z* Calcd. For C<sub>25</sub>H<sub>18</sub>N<sub>2</sub>OPt 556.0983 [M – H]<sup>+</sup>, Found 556.0977.

Pt-complex **1c**: <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, r.t.):  $\delta$  7.19-7.24 (m, 3H), 7.53 (d, J = 7.8 Hz, 4H), 7.64 (d, J = 7.8 Hz, 2H), 7.69 (d, J = 7.7 Hz, 2H), 7.94 (td, J = 7.7, 1.5 Hz, 2H), 9.38-9.51 (m, 2H). <sup>13</sup>C NMR (100 MHz, DMSO- $d_6$ , r.t.):  $\delta$  110.3 (C<sub>q</sub>), 120.9, 123.9 (C<sub>q</sub>), 124.9 (C<sub>q</sub>), 125.0 (C<sub>q</sub>), 125.1 (q,  $J_{C-F} = 270$  Hz), 125.5 (q,  $J_{C-F} = 31$  Hz), 125.5 (q,  $J_{C-F} = 3.7$  Hz, C<sub>q</sub>), 132.0 (C<sub>q</sub>), 133.2, 140.5 (C<sub>q</sub>), 143.3, 144.9, 155.0 (C<sub>q</sub>), 169.3, 177.6. FT-IR (ATR, cm<sup>-1</sup>): 3745, 3056, 2075, 1605, 1485, 1466, 1446, 1404, 1392, 1321, 1280, 1229, 1211, 1152, 1098, 1064, 1015, 839, 754, 736, 635, 600, 540, 521, 509, 483, 440. HR-MS (CH<sub>2</sub>Cl<sub>2</sub>): *m/z* Calcd. For C<sub>25</sub>H<sub>15</sub>F<sub>3</sub>N<sub>2</sub>Pt 594.0752 [M – H]<sup>+</sup>, Found 594.0766.



Figure S14a. <sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>, r.t.) of Pt-complex 1b.



Figure S14c. <sup>13</sup>C and DEPT 90 NMR spectra (100/125 MHz, DMSO-*d*<sub>6</sub>, r.t.) of Pt-complex 1b.







Figure S16a. <sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>, r.t.) of Pt-complex 1c.



**Figure S16b.** <sup>13</sup>C NMR spectrum (100 MHz, DMSO- $d_6$ , r.t.) of Pt-complex 1c.



Figure S16c. <sup>13</sup>C and DEPT 90 NMR spectra (100/125 MHz, DMSO-*d*<sub>6</sub>, r.t.) of Pt-complex 1c.



Figure S17. HR-MS spectrum (CH<sub>2</sub>Cl<sub>2</sub>) of Pt-complex 1c.

### Crystal structure and data of 1c (refinement special details)

A mixture of red and yellow crystals was obtained by allowing a saturated DMSO solution of **1c** to stand at r.t. for 3 d. The X-ray crystallographic analysis of the red crystal revealed the formation of two inequivalent stacked dimers  $(1c)_2$  with Pt(II)•••Pt(II) interactions (distances: 3.273(7) and 3.337(7) Å; Figure S18). Two DMSO molecules exist around the trifluoromethylphenyl groups of dimer  $(1c)_2$ , without coordination to the Pt(II) center, in the crystal. As a preliminary observation, only the red crystals emitted red luminescence, most probably derived from the metal-to-metal charge transfer (MMLCT) interactions of dimer  $(1c)_2$ .

Residual electron density remains closely on the platinum atoms, which is often caused by the effect of correction for heavy metal atom-based absorption.



Figure S18. Crystal structure of red crystal 1c (side and top views). Solvent molecules are omitted for clarity.



Figure S19. ORTEP drawing of red crystal 1c. The thermal ellipsoids are drawn at 50% probability.

Identification code	1c_red
Empirical formula	$C_{52}H_{36}F_6N_4OPt_2S$
Formula weight	1269.09
Temperature/K	93(3)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	8.85760(10)
b/Å	32.2146(4)
c/Å	31.0202(3)
α/°	90
β/°	92.3630(10)
γ/°	90
Volume/Å <sup>3</sup>	8843.90(17)
Z	8
$Q_{calc}g/cm^3$	1.906
µ/mm⁻¹	12.705
F(000)	4880
Crystal size/mm <sup>3</sup>	$0.15 \times 0.05 \times 0.05$
Radiation	CuK $\alpha$ ( $\lambda$ = 1.54184)
2⊖ range for data collection/°	3.956 to 154.012
Index ranges	$-9 \le h \le 11$ $-38 \le k \le 39$ $-39 \le 1 \le 38$
Reflections collected	85698
Independent reflections	17768 [ $R_{int} = 0.0452, R_{sigma} = 0.0314$ ]
Data/restraints/parameters	17768/52/1237
Goodness-of-fit on F <sup>2</sup>	1.126
Final R indexes $[I \ge 2\sigma(I)]$	$R_1 = 0.0433, wR_2 = 0.1140$
Final R indexes [all data]	$R_1 = 0.0470, wR_2 = 0.1157$
Largest diff. peak/hole / e Å-3	2.67/-1.40

Table S1. Crystal data and structure refinement for the red crystal of 1c.

The supplementary crystallographic data (CCDC 2269104) can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures.



A mixture of **PBA** (1.3 mg, 2.0 µmol) and Pt-complex **1a** (1.1 mg, 2.0 µmol) was ground for 1.5 min using an agate mortar and pestle.<sup>[S2]</sup> After the addition of H<sub>2</sub>O (1.0 mL) to the mixture, the suspended solution was centrifuged (14,800g, 10 min) and then filtered by a membrane filter (pore size: 200 nm) to give a clear orange solution of (**PBA**)<sub>*n*</sub>•(**1a**)<sub>*m*</sub>. The product structure was confirmed by UV-visible and DLS (d = 3.9 nm) analyses. After freeze drying, the concentration of encapsulated **1a** was estimated to be 0.1 mM by <sup>1</sup>H NMR analysis. In the same way, (**PBS**)<sub>*n*</sub>•(**1a**)<sub>*m*</sub>, (**ADA**)<sub>*n*</sub>•(**1a**)<sub>*m*</sub>, (**SDS**)<sub>*n*</sub>•(**1a**)<sub>*m*</sub>, and (**DTAC**)<sub>*n*</sub>•(**1a**)<sub>*m*</sub> were obtained in water from **1a** and the corresponding amphiphiles.



Figure S20. UV-visible spectra (H<sub>2</sub>O, r.t., 2.0 mM based on PBA) of  $(PBA)_n \cdot (1a)_m$ ,  $(PBA)_n$ , and 1a in CH<sub>2</sub>Cl<sub>2</sub>.



Figure S21a. <sup>1</sup>H NMR spectrum (500 MHz, D<sub>2</sub>O, r.t., 2.0 mM based on PBA) of (PBA)<sub>n</sub>•(1a)<sub>m</sub>.



Figure S21b. <sup>1</sup>H NMR spectrum (500 MHz, CD<sub>3</sub>OD, r.t.) of isolated (PBA)<sub>n</sub>•(1a)<sub>m</sub>.



Figure S22. a) DLS charts (H<sub>2</sub>O, r.t., 2.0 mM based on PBA) of (PBA)<sub>n</sub>•(1a)<sub>m</sub> and (PBA)<sub>n</sub>. b) Optimized structure of (PBA)<sub>30</sub>•(1a)<sub>16</sub> (MM calculation).



Figure S23. a) UV-visible spectra (H<sub>2</sub>O, r.t., 2.0 mM based on amphiphiles) of (PBA)<sub>n</sub>•(1a)<sub>m</sub>, (PBS)<sub>n</sub>•(1a)<sub>m</sub>, (AA)<sub>n</sub>•(1a)<sub>m</sub>, (ADA)<sub>n</sub>•(1a)<sub>m</sub>, (SDS)<sub>n</sub>•(1a)<sub>m</sub>, and (DTAC)<sub>n</sub>•(1a)<sub>m</sub>, and b) their normalized spectra (except for (SDS or DTAC)<sub>n</sub>•(1a)<sub>m</sub>).



Figure S24. Relative uptake efficiencies of various micelles toward 1a in water.



Figure S25a. Emission spectra (r.t.,  $\lambda_{ex} = 450 \text{ nm}$ ) of 1a in CH<sub>2</sub>Cl<sub>2</sub> (0.02 mM), solid 1a, ground solid 1a, and (PBA)<sub>n</sub>•(1a)<sub>m</sub> in water (2.0 mM based on PBA).



**Figure S25b.** UV-visible spectra (r.t., 0.02 mM) of a) **1a**, b) **1b**, c) **1c** in CH<sub>2</sub>Cl<sub>2</sub> and 1:1 DMSO/H<sub>2</sub>O, and d-f) their emission spectra (r.t.,  $\lambda_{ex} = 391$  nm), respectively.



Figure S26. Emission spectra (H<sub>2</sub>O, r.t.,  $\lambda_{ex} = 450$  nm, 2.0 mM based on amphiphiles) of  $(PBA)_n \bullet (1a)_m$ ,  $(PBS)_n \bullet (1a)_m$ ,  $(ADA)_n \bullet (1a)_m$ ,  $(AA)_n \bullet (1a)_m$ ,  $(SDS)_n \bullet (1a)_m$ , and  $(DTAC)_n \bullet (1a)_m$ .



**Figure S27.** Emission quantum yields (r.t.,  $\lambda_{ex} = 450$  nm, 2.0 mM based on amphiphiles) of various host-guest composites including **1a** in water.



**Figure S28.** Emission decay profiles (H<sub>2</sub>O, r.t.,  $\lambda_{ex} = 280$  nm,  $\lambda_{det} = 700$  nm, 2.0 mM based on amphiphiles) of (**PBA**)<sub>*n*</sub>•(**1a**)<sub>*m*</sub>, (**PBS**)<sub>*n*</sub>•(**1a**)<sub>*m*</sub>, and (**AA**)<sub>*n*</sub>•(**1a**)<sub>*m*</sub>.



**Figure S29.** a) UV-visible spectra (H<sub>2</sub>O, r.t., 2.0 mM based on amphiphiles) of  $(PBA)_n \cdot (1a)_m$ ,  $(PBA)_n \cdot (1b)_m$ , and  $(PBA)_n \cdot (1c)_m$ , and b) their normalized spectra.



Figure S30. Emission spectra (H<sub>2</sub>O, r.t.,  $\lambda_{ex} = 450$  nm, 2.0 mM based on PBA) of (PBA)<sub>n</sub>•(1a-c)<sub>m</sub>.



Figure S31a. Emission quantum yields (r.t.,  $\lambda_{ex} = 450 \text{ nm}$ ) of  $(PBA)_n \cdot (1a-c)_m$  in water (2.0 mM based on PBA) and ground solids 1a-c.



**Figure S31b.** CIE diagrams (r.t.,  $\lambda_{ex} = 450 \text{ nm}$ ) of a) (**PBA**)<sub>n</sub>•(**1a-c**)<sub>m</sub> in water (2.0 mM based on **PBA**) and b) ground solids **1a-c**.



Figure S32a. Emission spectra (r.t.,  $\lambda_{ex} = 391$  nm) of (PBA)<sub>n</sub>•(1a)<sub>m</sub> in 1.0:0-0.3 H<sub>2</sub>O/DMSO.



Figure S32b. UV-visible spectra (r.t.) of  $(PBA)_n \bullet (1a)_m$  in H<sub>2</sub>O and 1.0:0.3 H<sub>2</sub>O/DMSO.



Figure S32c. <sup>1</sup>H NMR spectra (400 MHz, r.t.) of  $(PBA)_n \bullet (1a)_m$  in a) D<sub>2</sub>O and b) 1.0:0.3 D<sub>2</sub>O/DMSO- $d_6$ .



A mixture of **PBA** (1.3 mg, 2.0  $\mu$ mol), **1a** (1.1 mg, 2.0  $\mu$ mol), and **BC** (1.0 mg, 2.0  $\mu$ mol) was ground for 1.5 min using an agate mortar and pestle.<sup>[S2]</sup> After the addition of H<sub>2</sub>O (1.0 mL) to the mixture, the suspended solution was centrifuged (14,800g, 10 min) and then filtered by a membrane filter (pore size: 200 nm) to give a clear orange solution of (**PBA**)<sub>n</sub>•(**1a**)<sub>m</sub>•(**BC**)<sub>p</sub>. The product structure was confirmed by UV-visible, DLS (d = 13 nm), and AFM (d = 14 nm) analyses. After freeze drying, the concentration of encapsulated **1a** and **BC** was estimated to be 0.4 and 0.6 mM, respectively, by <sup>1</sup>H NMR analysis.



Figure S33. UV-visible spectra (H<sub>2</sub>O, r.t., 2.0 mM based on PBA) of a)  $(PBA)_n \bullet (1a)_m \bullet (BC)_p$ , b)  $(PBA)_n \bullet (1a)_m \bullet (PC)_p$ , c)  $(PBA)_n \bullet (1a)_m \bullet (Cz)_p$ , d)  $(PBA)_n \bullet (1a)_m \bullet (BP)_p$ , e)  $(PBA)_n \bullet (1a)_m \bullet (Ant)_p$ , f)  $(PBA)_n \bullet (1a)_m \bullet (Cor)_p$ , and g)  $(PBA)_n \bullet (1a)_m \bullet (Per)_p$ .



Figure S34a. <sup>1</sup>H NMR spectrum (500 MHz, D<sub>2</sub>O, r.t., 2.0 mM based on PBA) of  $(PBA)_n \bullet (1a)_m \bullet (BC)_p$ .



Figure S34b. <sup>1</sup>H NMR spectrum (500 MHz, DMSO-*d*<sub>6</sub>, r.t.) of isolated (PBA)<sub>n</sub>•(1a)<sub>m</sub>•(BC)<sub>p</sub>.



**Figure S34c.** <sup>1</sup>H NMR spectra (400 MHz, D<sub>2</sub>O). of (**PBA**)<sub>*n*</sub>•(**BC**)<sub>*p*</sub> at r.t., 60 °C, and 80 °C.



Figure S34d. ESI-TOF MS spectrum (CH<sub>3</sub>OH) of (PBA)<sub>n</sub>•(1a)<sub>m</sub>•(BC)<sub>p</sub>.



Figure S35. Emission spectra (r.t., H<sub>2</sub>O,  $\lambda_{ex} = 450$  nm, 2.0 mM based on PBA) of a) (PBA)<sub>n</sub>•(1a)<sub>m</sub>•(BP, PC, BC, or Cz)<sub>p</sub> and b) (PBA)<sub>n</sub>•(1a)<sub>m</sub>•(Per, Ant, BC, or Cor)<sub>p</sub>.



Figure S36. Emission quantum yields (r.t., H<sub>2</sub>O,  $\lambda_{ex} = 450$  nm, 2.0 mM based on PBA) of  $(PBA)_n \bullet (1a)_m \bullet (BC, Cz, PC, BP, Cor, Ant, or Per)_p$ .



Figure S37. CIE diagram (r.t., H<sub>2</sub>O,  $\lambda_{ex} = 450$  nm, 2.0 mM based on PBA) of (PBA)<sub>n</sub>•(1a)<sub>m</sub> and (PBA)<sub>n</sub>•(1a)<sub>m</sub>•(BC)<sub>p</sub>.



Figure S38. Emission decay profiles (H<sub>2</sub>O, r.t.,  $\lambda_{ex} = 280$  nm,  $\lambda_{det} = 700$  nm, 2.0 mM based on **PBA**) of (**PBA**)<sub>n</sub>•(**1a**)<sub>m</sub>•(**BC**)<sub>p</sub> and (**PBA**)<sub>n</sub>•(**1a**)<sub>m</sub>.



Figure S39. DLS chart (H<sub>2</sub>O, r.t., 2.0 mM based on PBA) of (PBA)<sub>n</sub>•(1a)<sub>m</sub>•(BC)<sub>p</sub>.



Figure S40. a) AFM image (dry, r.t., mica) of  $(PBA)_n \bullet (1a)_m \bullet (BC)_p$  and b) the size and number distribution.



**Figure S41a.** Emission spectra (r.t.,  $\lambda_{ex} = 450 \text{ nm}$ ) of  $(\mathbf{PBA})_n \bullet (\mathbf{1a})_m \bullet (\mathbf{BC})_p$  in H<sub>2</sub>O (2.0 mM based on **PBA**) and a ground solid of a 1:1 mixture of **1a** and **BC**.



**Figure S41b.** Emission spectra (r.t.,  $\lambda_{ex} = 450$  nm) of solid  $(1a)_m \cdot (BC)_p$  obtained by evaporation of a CH<sub>2</sub>Cl<sub>2</sub> solution of 1a and BC, and solid 1a obtained by evaporation of a CH<sub>2</sub>Cl<sub>2</sub> solution of 1a.



**Figure S42.** a) UV-visible spectra (H<sub>2</sub>O, r.t., 2.0 mM based on **PBA**) of (**PBA**)<sub>*n*</sub>•(**1a**)<sub>*m*</sub>•(**BC**)<sub>*p*</sub> and products obtained by vigorous stirring a mixture of **PBA**, **1a**, and **BC** (1:1:1 molar ratio) in water for 5 h and b) their emission spectra (r.t., 2.0 mM based on **PBA**).



Yellow solid **PBA** (1.3 mg, 2.0  $\mu$ mol) was vigorously stirred in a H<sub>2</sub>O solution (1.0 mL) of Pt-complex **1a** (2.2 mg, 4.0  $\mu$ mol) at r.t. for 5 h. The resultant suspended solution was centrifuged (14,800g, 10 min) and then filtered by a membrane filter (pore size: 200 nm) to give a clear and colorless solution of (**PBA**)<sub>n</sub>•(**1a**)<sub>m</sub>. The product properties were revealed by UV-visible and emission analyses. In the same way, aqueous solutions of (**PBA**)<sub>n</sub>•(**1a**)<sub>m</sub> and (**PBA**)<sub>n</sub>•(**1c**)<sub>m</sub> were prepared by using red solids **1a** and **1c** (after grinding for 1.5 min), respectively.



Figure S43. UV-visible spectra (H<sub>2</sub>O, r.t., 2.0 mM based on PBA) of a) (PBA)<sub>n</sub>•(1a)<sub>m</sub> and b) (PBA)<sub>n</sub>•(1c)<sub>m</sub> prepared from PBA and 1a/1c via grinding or stirring.



**Figure S44.** Emission spectra (H<sub>2</sub>O, r.t., 2.0 mM based on **PBA**, left:  $\lambda_{ex} = 391$  nm, right:  $\lambda_{ex} = 450$  nm) of a) (**PBA**)<sub>n</sub>•(**1a**)<sub>m</sub> and b) (**PBA**)<sub>n</sub>•(**1c**)<sub>m</sub> prepared from **PBA** and **1a**/**1c** via grinding or stirring.



**Figure S45.** Emission spectra (r.t., left:  $\lambda_{ex} = 391$  nm, right:  $\lambda_{ex} = 450$  nm) of solids a) **1a**, b) **1b**, and c) **1c** obtained by evaporation of their solutions in various solvents (CH<sub>2</sub>Cl<sub>2</sub>, acetone, CH<sub>3</sub>OH, or DMSO).