Supporting Information

Novel Helical Assembly of a Pt(II) Phenylbipyridine Complex Directed by Metal–Metal Interaction and Aggregation-Induced Circularly Polarized Emission

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**Figure S8.** Dynamic light scattering (DLS) profile showing the intensity-averaged hydrodynamic radius of S-1 in toluene at 25 °C.

**Figure S9.** UV/vis absorption and CD spectra of S-1 (0.50 mmol L⁻¹) in toluene at 25 °C before heating.

**Figure S10.** (a) Time-dependent emission spectra of S-1 (0.50 mmol L⁻¹) in toluene at 25 °C before heating. (b) The plot of emission intensity at 820 nm vs t.

**Figure S11.** Photographs of (left) toluene solution and (right) chloroform solution of S-1 under irradiation of (top) room light and (bottom) UV (365 nm) light.

**Figure S12.** Photographs of solids of S-1 obtained by evaporation of (left) toluene solution and (right) chloroform solution under irradiation of (top) room light and (bottom) UV (365 nm) light.

**Figure S13.** ¹H NMR spectra of (a) solid A and (b) solid B dissolved in chloroform-d.

**Figure S14.** (a) AFM image of S-1 on mica. (b) Height profile on the white line of (a).

**Figure S15.** (a) AFM image of S-1 on HOPG. (b) Height profile on the white line of (a).

**References**

¹H and ¹³C NMR spectra of newly synthesized compounds

Calculated Structure of Pt(II)phenylbipyridine complex possessing bis(p-methoxyphenylisoxazolyl)phenylacetylene ligand
**General Information:** All reagents and solvents were of the commercial reagent grade and were used without further purification except where noted. Dry CH$_2$Cl$_2$, DMF, and triethylamine were obtained by distillation over CaH$_2$. $^1$H and $^{13}$C NMR spectra were recorded on a Varian mercury-300 spectrometer and JEOL JNM-ECA600 spectrometer at 25 °C in CDCl$_3$ and chemical shifts were reported as the delta scale in ppm relative to CHCl$_3$ ($\delta = 7.260$ for $^1$H and 77.3 for $^{13}$C). UV/vis absorption spectra were recorded on a JASCO V-560 spectrophotometer. Fluorescence spectra were recorded on a JASCO FP-6500 spectrofluorometer. Fluorescence quantum yields were recorded on a JASCO FP-6500 spectrofluorometer with an integrating sphere (JASCO, ILF-533, diameter 10 cm). CD spectra were recorded on a JASCO J-720W spectropolarimeter. IR spectra were recorded on JASCO FT/IR-420S spectrometer. ESI-Mass spectra were recorded on Thermo Scientific LTQ Orbitrap XL hybrid FTMS. Optical rotations were recorded on a JASCO DIP-370 polarimeter. UV/vis absorption, fluorescence, and CD spectra were measured using a conventional quartz cell (light path 1 cm) with temperature control. Elemental analyses were performed using CHN analyzer. Preparative separations were performed by silica gel gravity column chromatography (Silica Gel 60N (spherical, neutral)). Recycling preparative GPC-HPLC separations were carried out on JAI LC-908s using preparative JAIGEL-2H, 2H, 1H columns in series. Compounds 2, S- and $R$-3, and 5 were prepared according to the reported methods.

**Analysis of self-association by $^1$H NMR experiments:** Hyperbolic curves were obtained by plotting of compound concentrations vs $^1$H NMR chemical shifts ($\delta$) of the aromatic protons. The curve-fitting analysis of the plots was carried out on the basis of an isodesmic association model, which is a type of unlimited self-association where the addition of each successive monomer to polymer involves an equal association constant ($K_2 = K_3 = \ldots = K_i = K_E$). The fitting functions are given by equation 1 for NMR experiments. $\delta$ denotes apparent chemical shifts obtained from spectra; $\delta_m$ and $\delta_s$ are chemical shifts for a monomer and self-assembled species, respectively. $K_E$ is the association constant; and $c$ is the total concentration of a compound. The complexation-induced shift $\Delta \delta$ displays the difference between $\delta_m$ and $\delta_s$. 

S3
\[
(c) = \alpha + (\beta - \alpha) \left( 1 + \frac{1 - \sqrt{4K\varepsilon c + 1}}{2K\varepsilon c} \right)^{\frac{1}{2}}
\]  \hspace{1cm} (1)

**Determination of the CD dissymmetry factor** \(g_{\text{abs}}\) **and the CPL dissymmetry factor** \(g_{\text{lum}}\):  

The CD dissymmetry factors \(g_{\text{abs}}\) were defined as \(2\Delta\varepsilon/\varepsilon\) at the wavelength of the first Cotton effect (468 nm). \(\Delta\varepsilon\) and \(\varepsilon\) are the molar circular dichroism and the molar extinction coefficient, respectively.  

The CPL dissymmetry factors \(g_{\text{lum}}\) were defined as \(2\Delta I/I\) at the wavelength of the strongest CPL (530 nm). \(\Delta I\) and \(I\) are the CPL and fluorescence intensities, respectively.
Figure S1. (a) COSY and (b) NOESY spectra of S-1 at 298 K in chloroform-$d_1$. 
**Figure S2.** Non-linear curve fitting of S-1 using $^1$H NMR in chloroform-$d_1$ at 298 K. The solid curves were obtained by the fitting analysis.

**Table S1.** Aggregation-induced shifts of S-1 in chloroform-$d_1$ at 298 K.

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Figure S3. Energy minimized structure calculated by DFT method at B3LYP/LanL2DZ [Pt] + 6-31G(d) [C,H,N,O] level of Pt(II)phenylbipyridine complex possessing bis(p-methoxyphenylisoxazolyl)phenylacetylene ligand. The chiral alkyl chains of S-1 are replaced by methyl groups.
Figure S4. (a) Energy diagram of Pt(II)phenylbipyridine complex possessing bis(p-methoxyphenylisoxazolyl)phenylacetylene ligand calculated by TD-DFT at B3LYP/LanL2DZ [Pt] + 6-31+G(d,p) [C,H,N,O] level. (b) Calculated UV/vis absorption spectrum.
Figure S5. Excitation spectra of S-1 in chloroform at 25 °C. The concentration of the solution of S-1 are 0.49 (dotted line) and 5.17 (dashed and solid line) mmol L⁻¹. \( \lambda_{em} = 580 \) (dotted and dashed line) and 800 (solid line) nm.

Figure S6. CD spectra of S-1 in chloroform at 25 °C. The concentration of the solution of S-1 are 0.49 (dotted line) and 5.17 (solid line) mmol L⁻¹.
**Figure S7.** (a) UV/vis absorption (solid line) and CD (dotted line), and (b) emission spectra of S-1 (0.50 mmol L\(^{-1}\)) in toluene at 50 °C. \(\lambda_{\text{ex}} = 444\) nm.

**Figure S8.** Dynamic light scattering (DLS) profile showing the intensity-averaged hydrodynamic radius of S-1 in toluene at 25 °C.
Figure S9. UV/vis absorption (solid line) and CD (dotted line) spectra of S-1 (0.50 mmol L\(^{-1}\)) in toluene at 25 °C before heating.

Figure S10. (a) Time-dependent emission spectra of S-1 (0.50 mmol L\(^{-1}\)) in toluene at 25 °C before heating. (b) The plot of emission intensity at 820 nm vs t.
Figure S11. Photographs of (left) toluene solution and (right) chloroform solution of S-1 under irradiation of (top) room light and (bottom) UV (365 nm) light.

Figure S12. Photographs of solids of S-1 obtained by evaporation of (left) toluene solution and (right) chloroform solution under irradiation of (top) room light and (bottom) UV (365 nm) light.
Figure S13. $^1$H NMR spectra of (a) solid A and (b) solid B dissolved in chloroform-$d$. * indicates solvents and impurities.
**Figure S14.** (a) AFM image of S-1 on mica. The sample was prepared by spin-coating the toluene solution of S-1 after one heating-cooling cycle. (b) Height profile on the white line of (a).

**Figure S15.** (a) AFM image of S-1 on HOPG. The sample was prepared by spin-coating the toluene solution of S-1 after one heating-cooling cycle. (b) Height profile on the white line of (a).
References


5,5’-(5-ethynyl-1,3-phenylene)bis(3-((S)-3,7-dimethyloctyloxy)phenyl)isoxazole)
(S-4)
5,5’-(5-ethynyl-1,3-phenylene)bis(3-((R)-3,7-dimethyloctyloxy)phenyl)isoxazole)

(R-4)

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\[\text{(R-4)}\]
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(6-phenyl-2,2'-bipyridine){5,5'-(5-ethynyl-1,3-phenylene)bis(3-(4-((R)-3,7-dimethyloctyl oxy)phenyl)isoxazole)}platinum (R-1)
Calculated Structure of Pt(II)phenylbipyridine complex possessing
bis(p-methoxyphenylisoaxoly)phenylacetylene ligand

![Chemical structure diagram]

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