

Electronic Supporting Information for

Photoexcited State Chirality Transfer. Hidden Tunability of Circularly Polarized Luminescent Binaphthyl-Anthracene Tandem Molecular Systems

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Experimental details

General methods

Compounds (*R*)-**1**, (*S*)-**1**, (*R*)-**2** and (*S*)-**2** were purchased from Sigma-Aldrich Japan (Tokyo, Japan). Chloroform (CHCl₃) and N,N-dimethylformamide (DMF) used for crystallisation and optical measurements was purchased from Wako Pure Chemical Industries (Osaka, Japan).

Measurement of the CPL and photoluminescence spectra

Photoluminescence (PL) spectra and absolute photoluminescence (PL) quantum yields of all samples in DMF were recorded on an absolute PL quantum yield measurement system (Hamamatsu Photonics C9920-02, Hamamatsu, Japan) under air atmosphere at room temperature. The DMF solutions of (*R*)-**1** and (*R*)-**2** (1.0×10^{-4} M) were excited at 350 nm and the pass length is 10 mm.

The CPL and PL spectra in DMF solution were measured using a JASCO CPL-200 spectrofluoropolarimeter (Tokyo, Japan) at room temperature ($\approx 25^\circ\text{C}$). The outline of optics used in the instrument adopts a scattering angle of 0° under excitation of unpolarised, monochromated incident beam with air-cooled 150-W Xenon light source. Bandwidths for excitation and emission for highly emissive (*R*)-**1** and (*S*)-**1** were 10 nm/10 nm, respectively. Bandwidths for weakly emissive (*R*)-**2** and (*S*)-**2** should be $3000 \mu\text{m}/3000 \mu\text{m}$, respectively, due to the extremely quantum efficiency. DMF solutions of 1.0×10^{-4} M were excited at 340

nm for **1** and 330 nm for **2**. Pathlength was commonly 2.0 mm, allowing 63–70% transmittance at 340 nm for **1** and 330 nm for **2**. To obtain improved CPL/PL spectra without any no numerical smoothing operations, we chose slow scanning speed with 50 nm min⁻¹, a long time constant of PMT of 8 sec and 4–8 time acquisitions.

Measurement of CD and UV-Vis absorption spectra

The circular dichroism (CD) and UV-Vis absorption spectra of (*R*)-**1**, (*S*)-**1**, (*R*)-**2** and (*S*)-**2** in DMF solution (1.0×10^{-4} M) were measured using a JASCO J-820 spectropolarimeter at 25 °C. The pass length of UV-grade fused quartz cuvette is 2.0 mm.

Theoretical calculations

The geometry of (*R*)-**2** was optimised using the hybrid density functional theory (B3LYP functional).¹ The excitation energies and rotational strengths of the geometry-optimised molecules were calculated using the time-dependent density functional theory² with the B3LYP functional. In all the calculations, the cc-pVDZ basis set was used.³ The program Gaussian03⁴ was used for quantum chemical calculations.

References

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