Electronic Supporting Information for

Solvent-sensitive Signs and Magnitudes of Circularly Polarised Luminescence and Circular Dichroism Spectra: Probing Two Phenanthrenes as Emitters Endowed with BINOL Derivatives

Shoma Nakanishi, Nobuyuki Hara, Natsuki Kuroda, Nobuo Tajima, Michiya Fujiki and Yoshitane Imai

Department of Applied Chemistry, Faculty of Science and Engineering, Kindai University, 3-4-1 Kowakae, Higashi-Osaka, Osaka 577-8502, Japan.
Computational Materials Science Center, National Institute for Materials Science 1-2-1 Sengen, Tsukuba, Ibaraki 305-0047, Japan.
Graduate School of Materials Science, Nara Institute of Science and Technology, Takayama, Ikoma, Nara 630-0192, Japan.

Correspondence to: (Y.I.) y-imai@apch.kindai.ac.jp. (M.F.) fujikim@ms.naist.jp.

S1
Table of contents

Fig. S1 Simulated CD spectra of (R)-2a in MeOH and in vacuo using TD-DFT .......................S3
Fig. S2 CPL and PL spectra of (R)-2c in MeOH.......................................................................S4
Fig. S3 CPL and PL spectra of (R)-2d in DMF .........................................................................S4
Fig. S4 CPL and PL spectra of (R)-2a in co-solvents....................................................................S5
Fig. S5 CD and UV absorption spectra of (R)-2a in co-solvents.............................................S6
Fig. S1. CD spectra of (R)-2a calculated with or without solvent effect, using the methods of calculations for obtaining Fig. 6. MeOH/vacuo (black line) means the CD spectrum is simulated with the solvent effect of MeOH, and this calculation uses the gas phase geometry. MeOH/MeOH (red line) and vacuo/vacuo (green line) means the CD spectra are simulated with or without MeOH solvent effect, respectively, with the molecular geometries determined for the respective media.
Fig. S2. CPL (upper blue plot) and PL (lower red plot) spectra of (R)-2c in MeOH. [Conc]₀ = 1.0 × 10⁻⁴ M. λₑₓ = 300 nm. Path length = 10 mm. The \( g_ₑ m \) value is 1.6 × 10⁻³ at 361 nm.

Fig. S3. CPL (upper blue plot) and PL (lower red plot) spectra of (R)-2d in DMF. [Conc]₀ = 1.0 × 10⁻⁴ M. λₑₓ = 300 nm. Path length = 10 mm. The \( g_ₑ m \) value is 1.9 × 10⁻³ at 361 nm.
Fig. S4. CPL (upper blue plot) and PL (lower red plot) spectra of (R)-2a in (a) CHCl₃/DMF (2/1, v/v), (b) CHCl₃/DMF (1/1, v/v), and (c) CHCl₃/DMF (1/2, v/v). [Conc]₀ = 1.0 × 10⁻⁴ M. λₑₓ = 300 nm. Path length = 10 mm. The gₑₘ value is -1.0 × 10⁻⁴ at 358 nm for CHCl₃/DMF (2/1, v/v), -0.2 × 10⁻⁴ at 362 nm for CHCl₃/DMF (1/1, v/v), and -1.5 × 10⁻⁴ at 356 nm for CHCl₃/DMF (1/2, v/v).
Fig. S5. CD (upper plot) and UV absorption (lower plot) spectra of (R)-2a in (a) CHCl₃/DMF (2/1, v/v), (b) CHCl₃/DMF (1/1, v/v), and (c) CHCl₃/DMF (1/2, v/v). Conc. = 1.0 × 10⁻⁴ M. Path length = 1 mm.