Supporting Information

Chiral 1,2-Subnaphthalocyanines

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I. ^1H NMR spectra of **1c**, **2c**, **1d**, and **2d**

Figure S1. ^1H NMR spectra of (a) **1c** and (b) **2c** in CDCl_3 .

Figure S2. ^1H NMR spectra of (a) **1d** and (b) **2d** in CDCl_3 .

II. Crystal packing diagrams and crystallographic data

Table S1. Crystallographic data of **1c**, **2c**, and **1dFr1**

Compound	1c	2c	1dFr1
Empirical formula	C ₄₂ H ₂₃ BN ₆ O	C ₄₂ H ₂₃ BN ₆ O	C ₄₈ H ₂₇ BN ₆ OBrCl
Formula weight	638.49	638.49	829.93
Temperature (K)	173(2)	173(2)	100(2)
Wavelength (Å)	0.71070	0.71070	0.71073
Crystal system	<i>P</i> 2 ₁ /n	<i>P</i> 2 ₁ /n	<i>P</i> 2 ₁ 2 ₁ 2 ₁
Space group	monoclinic	monoclinic	orthorhombic
Unit cell dimensions	<i>a</i> = 10.304(6) Å	<i>a</i> = 11.572(7) Å	<i>a</i> = 10.977(3) Å
	<i>b</i> = 17.641(10) Å, <i>β</i> = 91.985(8)°	<i>b</i> = 19.432(10) Å, <i>β</i> = 110.876(8)°	<i>b</i> = 17.802(4) Å
	<i>c</i> = 16.769(10) Å	<i>c</i> = 14.691(8) Å	<i>c</i> = 38.101(9) Å
Volume (Å ³)	3046(3)	3087(3)	7445(3)
Z	4	4	8
Density (calc) (g/cm ³)	1.392	1.374	1.481
μ (mm ⁻¹)	0.086	0.085	1.225
F(000)	1320	1320	3376
Crystal size (mm ³)	0.26 x 0.20 x 0.07	0.23 x 0.15 x 0.06	0.40 x 0.08 x 0.05
θ for data collection	3.0 to 27.4	3.1 to 27.4	1.26 to 25.52
Index ranges	-13<= <i>h</i> <=13, -22<= <i>k</i> <=22, -21<= <i>l</i> <=21	-14<= <i>h</i> <=14, -25<= <i>k</i> <=25, -18<= <i>l</i> <=18	-13<= <i>h</i> <=13, -21<= <i>k</i> <=13, -44<= <i>l</i> <=46
Reflection collected	43770	44631	36846
Independent reflections	6895	6951	13804
Completeness	0.966	0.997	0.997
Absorption correction	numerical	numerical	empirical
Max. and min. transmission	0.983, 0.979	0.995, 0.991	0.9413, 0.6399
Refinement method	SHELXL-97	SHELXL-97	SHELXL-97
Data/restraints/parameters	6895/0/474	6951/0/474	13804/276/1055
Goodness-of-fit on <i>F</i> ²	0.966	1.002	0.988
Final <i>R</i> indices [<i>I</i> >2σ(<i>I</i>)]	0.0667	0.0707	0.0845
<i>wR</i> 2 indices (all data)	0.1224	0.1936	0.2761
Large diff. peak and hole	0.90, -0.81	0.71, -0.64	0.900, -0.757
Absolute structure parameter			0.015(17)
Diffractometer	Rigaku Saturn	Rigaku Saturn	Bruker APEX II
CCDC number	828217	828218	828219

Figure S3. Crystal packing diagrams of (a) 1c and (b) 2c.

Figure S4. Crystal packing diagram of 1dFr1.

III. Chiral-HPLC chromatograms of 1c and 2c

Figure S5. Chiral-HPLC chromatograms of 1c (top) and 2c (bottom) detected by absorbance at 520 nm. Each chromatogram is normalized to the maximum intensity. The enantiomers of 1c were separated by recycling for several times.

IV. Band deconvolution analyses

Figure S6. Absorption (bottom) and MCD (middle) spectra of **1c**, and CD (top) spectrum of **1cFr1** in CHCl_3 . Deconvoluted Gaussian curves and the simulated spectra of **1c** are shown by the gray or blue lines and the blue dashed line. The Q_{00} -bands are denoted by the blue Gaussian curves.

Figure S7. Absorption (bottom) and MCD (middle) spectra of **2c**, and CD (top) spectrum of **2cFr1** in CHCl_3 . Deconvoluted Gaussian curves and the simulated spectra of **2c** are shown by the gray or blue lines and the blue dashed line. The Q_{00} -bands are denoted by the blue Gaussian curves.

V. Theoretical CD spectra and calculated rotational strengths

Figure S8. Theoretical absorption and CD spectra of the clockwise isomer (left) and the anti-clockwise isomer (right) of **1** based on TDDFT calculation.

Figure S9. Theoretical absorption and CD spectra of the clockwise isomer (left) and the anti-clockwise isomer (right) of **2** based on TDDFT calculation.

VI. Absorption, MCD, and CD spectra of 1d and 2d

Figure S10. Absorption (bottom) and MCD (middle) spectra of **1d** (left) and **2d** (right) in CHCl_3 , and CD (top) spectra of **1dFr1** and **2dFr1** (blue) and **1dFr2** and **2dFr2** (red) in CHCl_3 . Fluorescence spectra in CHCl_3 are shown as dashed lines (bottom).

VII. Full list of authors of the reference 21

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