Electronic Supporting Information (ESI) for

Stereo-Chemical Analysis of Racemization of a Chiral Bipyridine

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Figure S1. VCD (upper) and IR (lower) spectra of CHIRABIPY/$CuCl_2$ (Precipitates) in $CDCl_3$ solution.

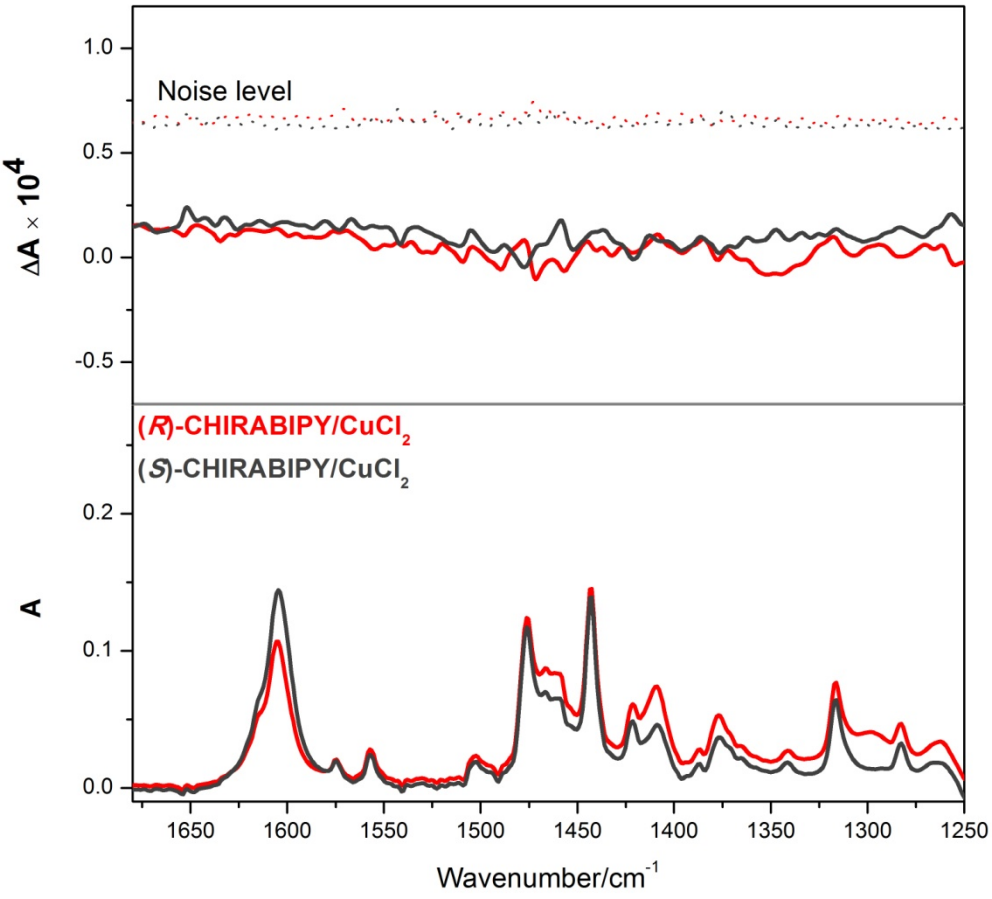

Table S1. B3LYP/6-311++G Optimized Structure (Atom Coordinates) of (*R*)-CHIRABIPY**

C	5.58165000	0.37859400	0.20927200
C	4.64165800	1.40505300	0.14964200
N	3.32585100	1.19757300	0.04839800
C	2.87821700	-0.06986600	0.00106000
C	3.75235200	-1.16471000	0.05522000
C	5.11870400	-0.93447200	0.16050700
C	1.40334700	-0.26874100	-0.11390200
N	0.95914900	-1.53503300	-0.16585000
C	-0.35793500	-1.74012400	-0.27442500
C	-1.30094100	-0.71751500	-0.33767500
C	-0.83725200	0.60854400	-0.27550900
C	0.52998700	0.82685100	-0.16524500
C	-2.78371000	-0.92173300	-0.49392100
C	-3.28511000	1.14998100	-0.48646000
C	-1.86723000	1.72403800	-0.31794500
C	-3.25799400	0.06966300	-1.60422500
C	-3.56389800	-0.01154800	0.53865500
C	-5.05395300	-0.37564100	0.60586800
C	-3.03379700	0.11198500	1.96759900
H	6.63742700	0.60583700	0.29081100
H	4.96136400	2.44279300	0.18462100
H	3.35093800	-2.16750400	0.01450100
H	5.81187900	-1.76693300	0.20372900
H	-0.68084100	-2.77783100	-0.31635400
H	0.93466300	1.82952700	-0.11559400
H	-3.06025700	-1.97592800	-0.56315300
H	-4.02986000	1.94693800	-0.55235000
H	-1.63948500	2.40130400	-1.14879400
H	-1.79423200	2.32547900	0.59494900
H	-4.24649300	-0.17011500	-1.99123900
H	-2.57477500	0.23013100	-2.44122900
H	-5.18985100	-1.31899600	1.14438700
H	-5.60473400	0.39913100	1.14899100
H	-5.51715400	-0.48370100	-0.37595400
H	-1.97242900	0.35604700	2.01885500
H	-3.58230600	0.89206400	2.50603900
H	-3.18342200	-0.82817800	2.50885300

Table S2. B3LYP/6-311++G Calculated Absolute Energy of (*R*)-CHIRABIPY**

	Gibbs free energy(hartree)
(*R*)- CHIRABIPY	-768.069283

Figure S2. Packing Diagram of the Structure of (*R/S*)-CHIRABIPY/Pyromellitic Acid Co-Crystal

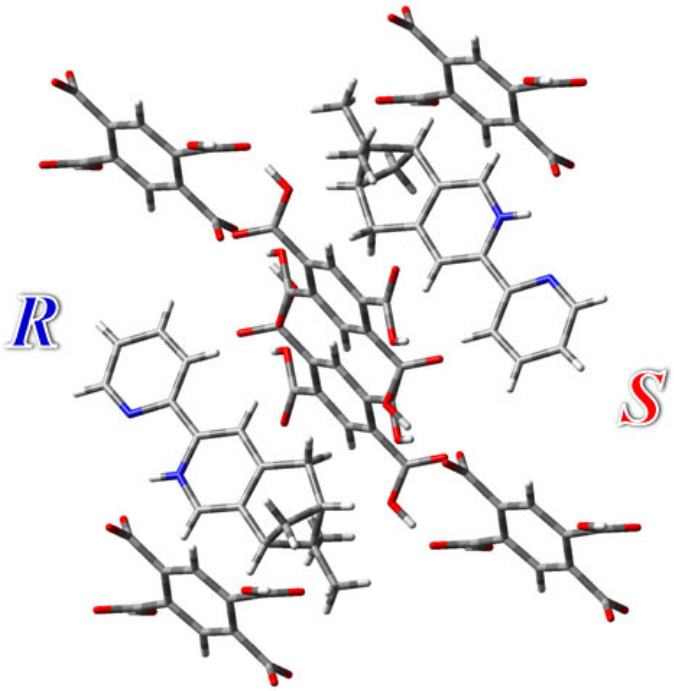

Table S3. Crystal Data of (*R/S*)-CHIRABIPY/Pyromellitic Acid Co-Crystal:

Crystal data

$C_{27}H_{24}N_2O_8$	γ = 82.960 (4)°
M_r = 504.48	V = 1173.7 (4) Å^3
Triclinic, P1	Z = 2
a = 7.2917 (15) Å	Mo Kα radiation, λ = 0.71073 Å
b = 10.673 (2) Å	μ = 0.11 mm^{-1}
c = 15.371 (3) Å	T = 291 K
α = 81.460 (4)°	0.12 × 0.11 × 0.10 mm
β = 87.501 (4)°	

Data collection

Bruker Smart Aepex CCD diffractometer	4041 independent reflections
Absorption correction: Multi-scan *SADABS*,Bruker,2000	3395 reflections with $I > 2\sigma(I)$
T_{min} = 0.987, T_{max} = 0.989	R_{int} = 0.041
5825 measured reflections	

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.077	0 restraints
$wR(F^2)$ = 0.180	H-atom parameters constrained
S = 1.22	$\Delta\rho_{max}$ = 0.46 e Å^{-3}
4041 reflections	$\Delta\rho_{min}$ = −0.30 e Å^{-3}
336 parameters	