

Supporting Information

Hydrogen-Bond-Stabilized Chiral Tetrakis Eu(III) Complex with Strong Circularly Polarized Luminescence

Kun Qian,^a Blanka Klepetářová,^b Petr Bouř,^b and Tao Wu^{*b}

^a College of Pharmacy, Jiangxi University of Chinese Medicine, Nanchang, 330006, P. R. China

^b *Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences, Flemingovo náměstí 2, 16610 Prague, Czech Republic*

E-mail: tao.wu@uochb.cas.cz

Table S1. Crystallographic data of $\text{ImH}^+[\text{Eu}((-)\text{-hfbc})_4]^-$ at room temperature

Crystallographic Data	
empirical formula	$\text{C}_{59}\text{H}_{61}\text{EuF}_{28}\text{N}_2\text{O}_8$
formula weight	1610.05
temperature (K)	293(2)
crystal system	orthorhombic
space group	$P2_12_12_1$
a, b, c (Å)	15.0718(4), 19.6057(5), 22.3568(6)
α, β, γ (deg)	90, 90, 90
Volume (Å ³), Z	6606.3(3), 4
$F(0\ 0\ 0)$	3232.0
crystal size (mm)	0.1×0.1×0.02
ϑ range for data collection (deg)	5.996 to 144.24
limiting indices	$-18 \leq h \leq 18, -20 \leq k \leq 24, -27 \leq l \leq 27$
tot., uniq. data, R (int)	78544, 4504, 0.072
observed data [$I > 2\sigma(I)$] 3644	12771
data/restraints/parameters	12771/42/884
R indices, goodness-of-fit	$R_1 = 0.0432, wR_2 = 0.1059, S = 0.946$
CCDC	2450565

Table S2. Crystallographic data of $\text{Na}^+[\text{Eu}((-)\text{-hfbc})_4]^-$ at room temperature

Crystallographic Data	
empirical formula	$\text{C}_{58}\text{H}_{59}\text{EuF}_{28}\text{NNaO}_8$
formula weight	1605
temperature (K)	293(2)
crystal system	orthorhombic
space group	$P2_12_12_1$
a, b, c (Å)	13.0593(4), 20.8865(6), 24.0412(7)
α, β, γ (deg)	90, 90, 90
Volume (Å ³), Z	6557.6(3), 4
$F(0\ 0\ 0)$	3216.0
crystal size (mm)	0.1×0.02×0.02
ϑ range for data collection (deg)	5.604 to 136.476
limiting indices	$-15 \leq h \leq 15, -25 \leq k \leq 24, -28 \leq l \leq 28$
tot., uniq. data, R (int)	87615, 4504, 0.085
observed data [$I > 2\sigma(I)$] 3644	11851
data/restraints/parameters	11851/2095/875
R indices, goodness-of-fit	$R_1 = 0.0397, wR_2 = 0.1009, S = 0.938$
CCDC	2450564

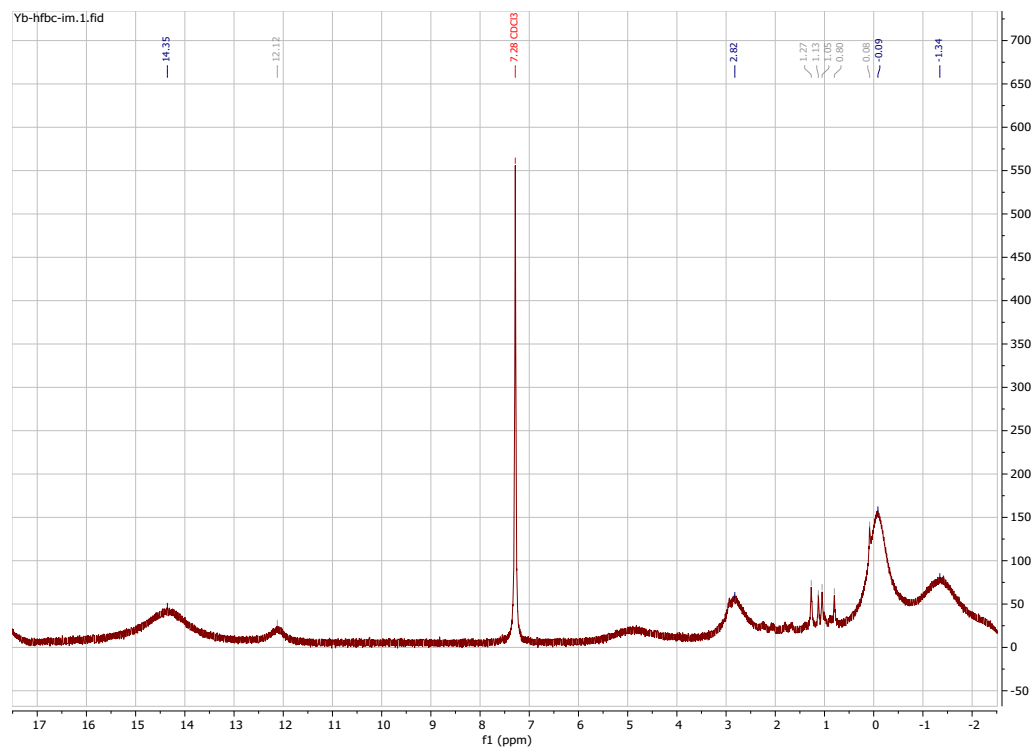


Fig. S1. ^1H NMR (CDCl_3) spectrum of the complex $\text{ImH}^+[\text{Yb}((+)\text{-hfbc})_4]^-$.

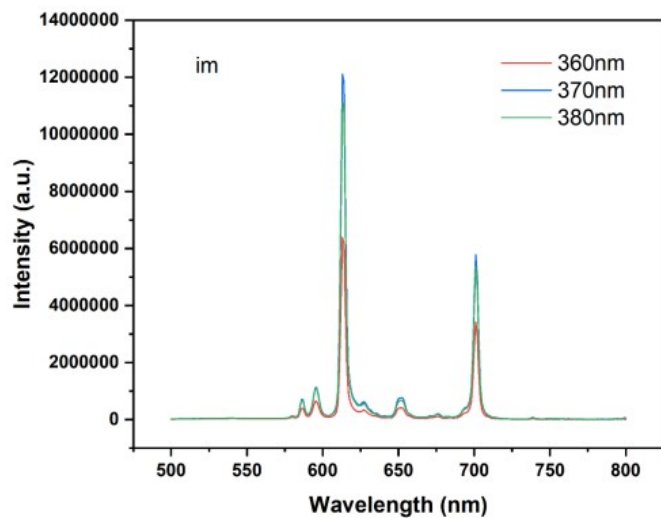


Fig. S2. Emission spectrum of complex $\text{ImH}^+[\text{Eu}((-)\text{-hfbc})_4]^-$ in 2 mM CHCl_3 solution under excitation at 360, 370, and 380 nm. The most intense emission was obtained with $\lambda_{\text{ex}} = 370$ nm.

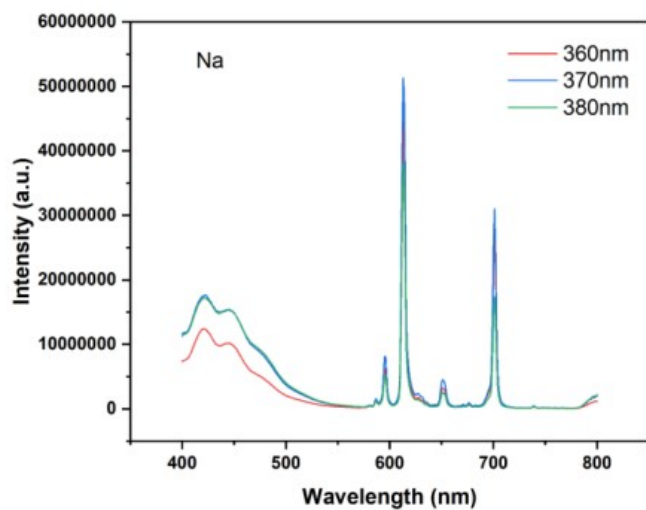


Fig. S3. Emission spectrum of complex $\text{Na}^+[\text{Eu}((-)\text{-hfbc})_4]^-$ in 2 mM CHCl_3 solution under excitation at 360, 370, and 380 nm. The most intense emission was obtained with $\lambda_{\text{ex}} = 370$ nm.

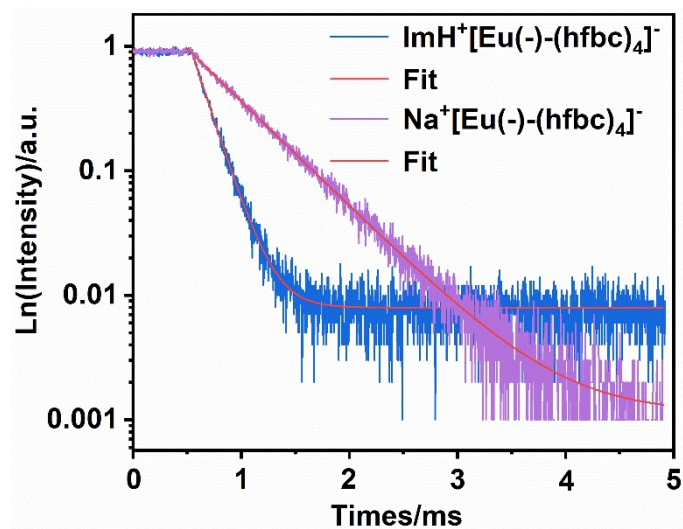


Fig. S4. Emission decay curves of complex $\text{ImH}^+[\text{Eu}((-)\text{-hfbc})_4]^-$ and $\text{Na}^+[\text{Eu}((-)\text{-hfbc})_4]^-$ in 2 mM CHCl_3 solution ($\lambda_{\text{ex}} = 370$ nm). And the red curves indicated the fit curves. The emission lifetimes are 0.16 ms and 0.51 ms, respectively.

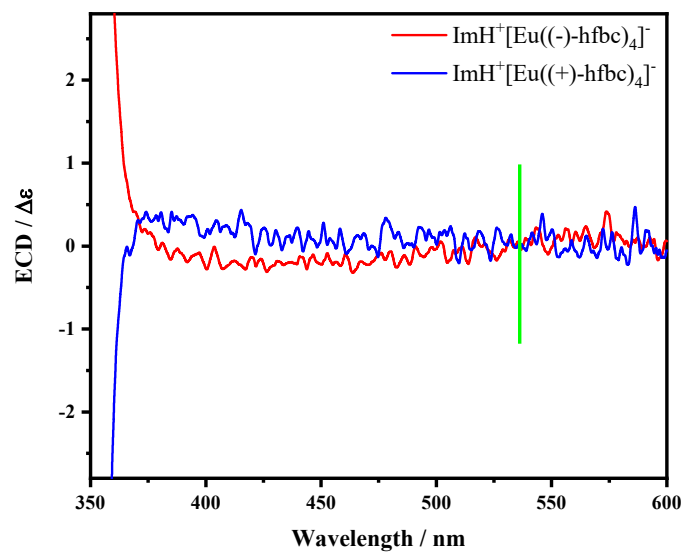


Fig. S5. ECD spectra of $\text{ImH}^+[\text{Eu}((+/-)\text{-hfbc})_4]^-$ enantiomer complexes (2 mM) in CHCl_3 , with the excitation laser line (532 nm) marked.

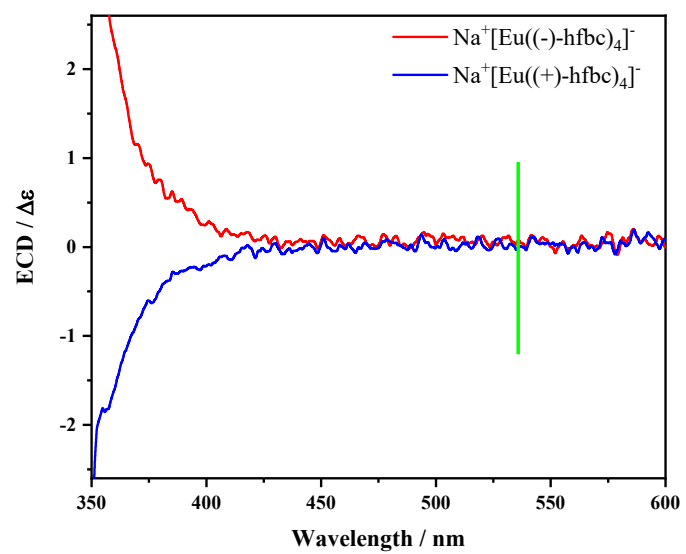


Fig. S6. ECD spectra of Na⁺[Eu((+/-)-hfbc)₄]⁻ enantiomer complexes (2 mM) in CHCl₃, with the excitation laser line (532 nm) marked.