Electronic Supplemental information

Experimental

Synthesis of the Δ-Cs[Ln ((+)-hfbc)₄] Complexes

A series of Δ-Cs-Ln complexes (Ln=La, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu) were obtained by the reported method¹⁰⁻¹⁵.

Measurements

VCD and IR spectra were measured with a PRESTO-S-2007 spectrometer (JASCO, Co.). The special instrument was developed for VCD measurements, being implemented with the shuttle system. A CDCl₃ solution of a complex (ca.0.01~ 0.03 M) was injected into a cell with BaF₂ windows of 150 μm optical length. The signal was accumulated during 5000 scans (ca. 50 minutes) for each complex with the resolution of 4 cm⁻¹. The molar absorbance of the IR spectra was adjusted below 1.0 for the optimal measurements.
DFT Computation

The IR and VCD spectra of the Cs-Lu complex were theoretically calculated by the use of Gaussian 09 program. VCD intensities were determined by the vibrational rotational strength and magnetic dipole moments, which were calculated by the magnetic field perturbation (MFP) theory formulated using magnetic field gauge-invariant atomic orbitals. The calculated intensities were converted to Lorentzian bands with 4 cm⁻¹ half-width at half-height. Geometry optimization was performed at the DFT level (B3LYP functional with Stuttgart ECP and Cs and 6-31G(d) for other atoms) for Lu(Figure S2). The observed spectra were assigned on the basis of the animations of molecular vibration with Gauss view 5.08 (Gaussian Inc.).
Figure S2. The optimized (top view) structure of the Δ-SAPR-8(C₄) Cs-Lu
Figure S3  The DFT calculated IR and VCD spectra of Δ-Cs-Lu
a) 1800-1300 cm$^{-1}$ and b) 1780 -1660 cm$^{-1}$