Electronic Supplementary Information

Dibenzo-diaza-30-crown-10-appended bis(zinc porphyrin) tweezers: synthesis and crown-assisted chiroptical behavior

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Cooperative association model of association constant (K_a) of **1**[28]

$$\mathbf{1} + \mathbf{1} \overset{K_2}{\rightleftharpoons} \mathbf{1}_2$$

$$\mathbf{1} + \mathbf{1}_{i-1} \overset{K_i = K_a}{\rightleftharpoons} \mathbf{1}_i \qquad \text{with } K_2 \neq K_3 = K_4 = \cdots\cdots\cdots = K_i = K_a$$

The concentration dependency of the chemical shift of N-CH_3 presented in Fig. 1, can now be described with Equation (1) and gives the association constants K_a and dimerization constant K_2.

$$\frac{(1-P_f)^{1/2}}{(2P_f - 1)c^{1/2}} = {K_2}^{1/2} + K_a \frac{P_f\left[(1-P_f)c\right]^{1/2}}{2P_f - 1} \qquad (1)$$

$$\text{with} \quad P_f = \frac{\delta_a - \delta_{obs}}{\delta_a - \delta_m}$$

where P_f: the population fraction of free N-CH_3;

c: total concentration of **1** (M);

δ_a: chemical shift of the fully associated state (2.01 ppm, c = 4.0 x 10^{-2} M);

δ_m: chemical shift of the monomer (2.86 ppm, c = 5.0 x 10^{-5} M);

δ_{obs}: observed chemical shift.

Measurements

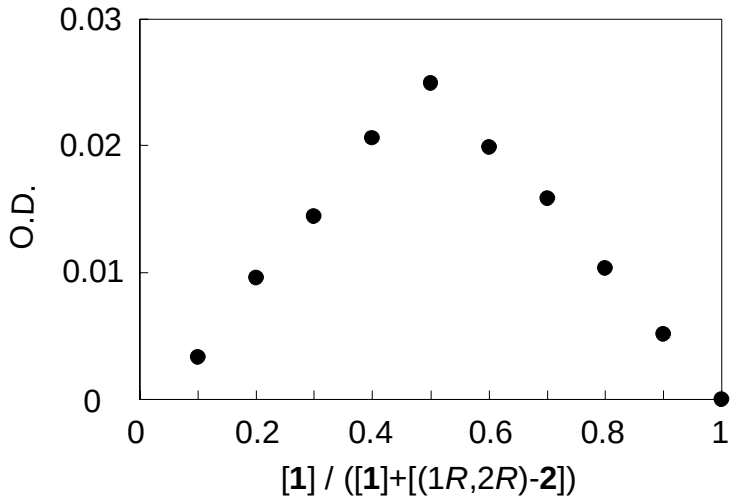

Fig. S1 A Job Plot for the complex formation between **1** and (1*R*,2*R*)-**2**. The total concentration was kept at 2.0 μM and the absorption intensity was monitoring by UV–Vis spectroscopy in CH_2Cl_2-MeCN at 25 ºC.

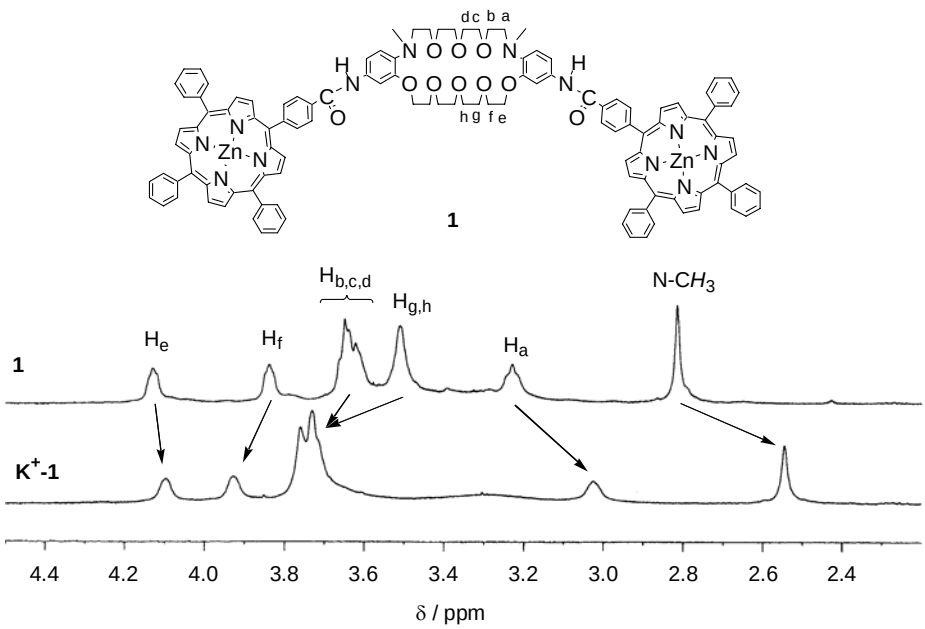

Fig. S2 ^{1}H NMR of crown ether region of **1** (a) and K^+-**1** complex (b) in CD_2Cl_2-CD_3CN (4:1 v/v) at 23 ºC. The K^+-**1** complex solution was obtained after solid[$KClO_4$] – liquid[1.0 mM of **1** CD_2Cl_2-CD_3CN (4:1 v/v)] two-phase extraction.

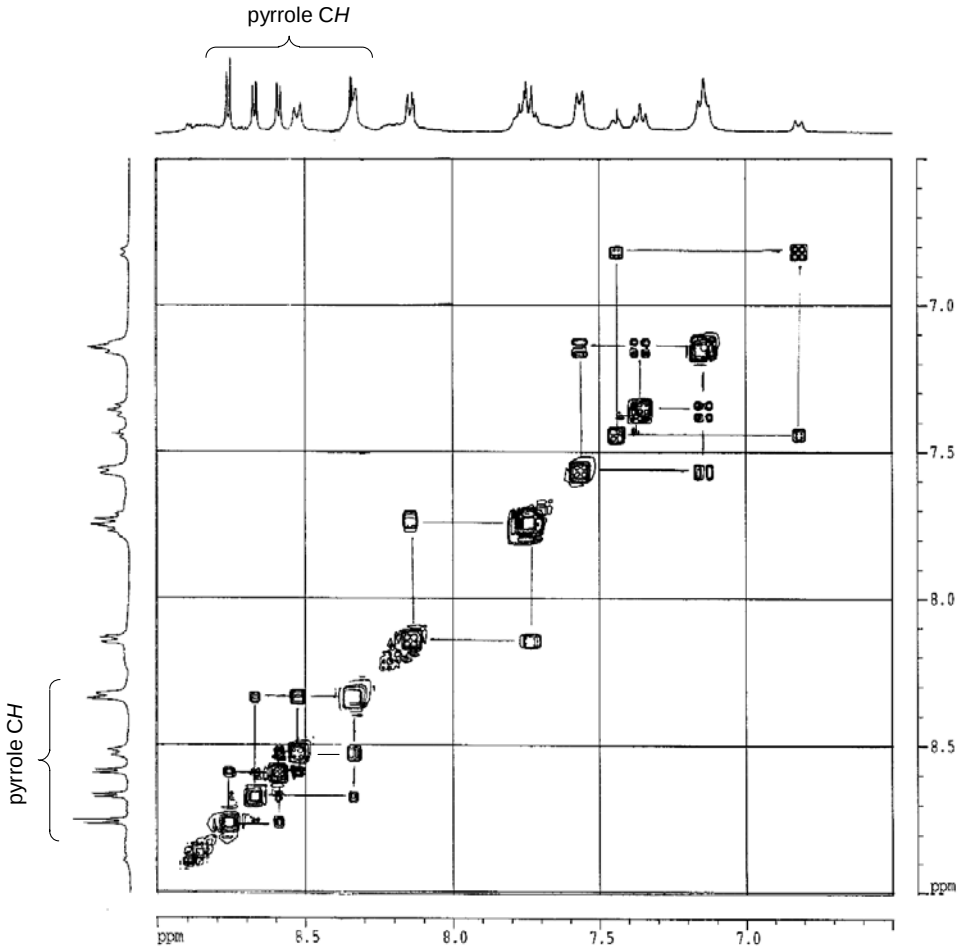

Fig. S3 2D COSY spectrum of K^+-**1** complex. The solution was obtained after solid[$KClO_4$] – liquid[1.0 mM of **1** CD_2Cl_2-CD_3CN (4:1 v/v)] two-phase extraction.

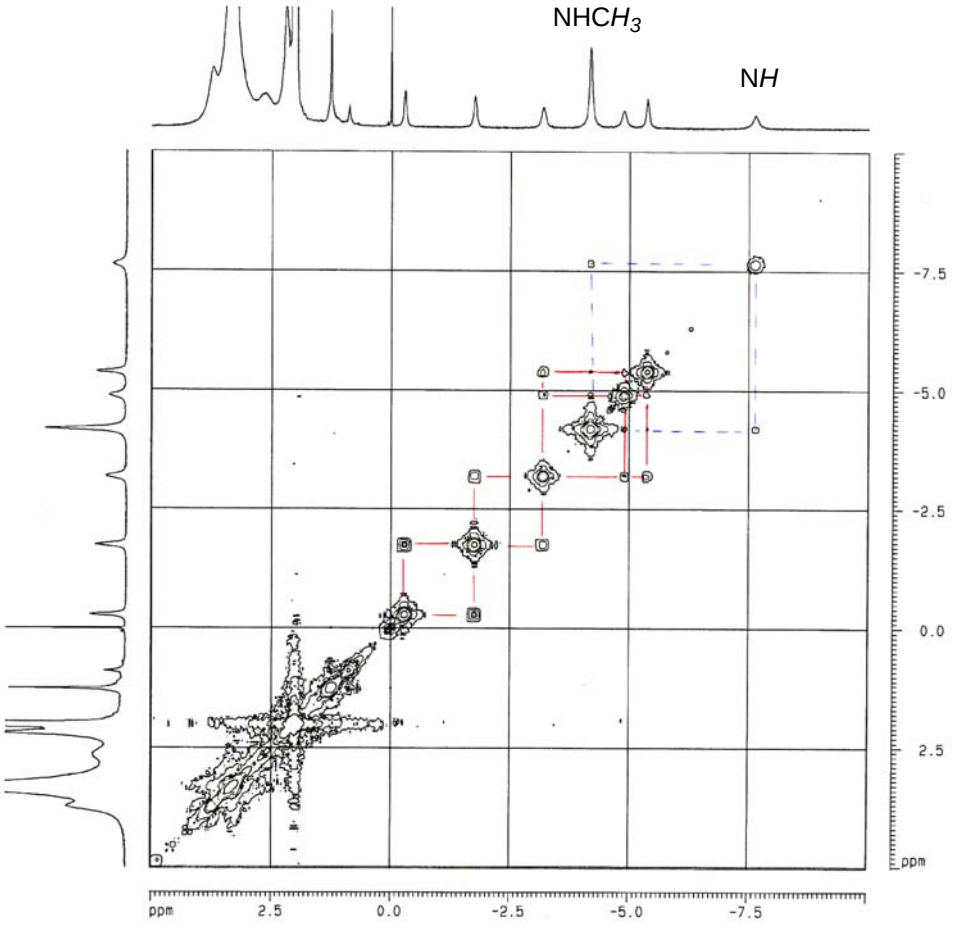

Fig. S4 2D COSY spectrum of K^+-**1**-(1*R*,2*R*)-**2** complex in CD_2Cl_2-CD_3CN (4:1 v/v) at 23 ˚C. The solution was obtained after solid[$KClO_4$] – liquid[10 mM of **1** and 5 mM of (1*R*,2*R*)-**2** in CD_2Cl_2-CD_3CN (4:1 v/v)] two-phase extraction.

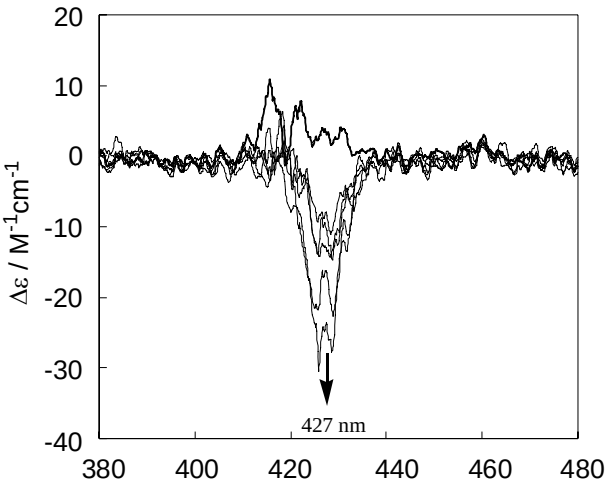

Fig. S5 CD spectral changes of **1** upon adding L-Trp-OMe in CH_2Cl_2 at 25 ˚C. [**1**] = 13 μM. Optical length = 0.2 cm.