Electronic Supplementary Information

Solid-State Self-Inclusion Complexation Behaviour of a Pillar[5]arene-Based Host–Guest Conjugate

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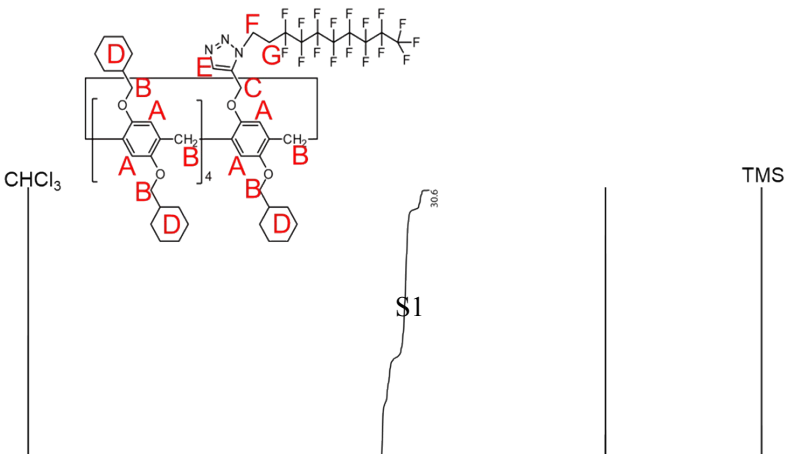


Fig. S1 ^{1}H NMR spectrum of **1d** in $CDCl_3$ at 25 °C.

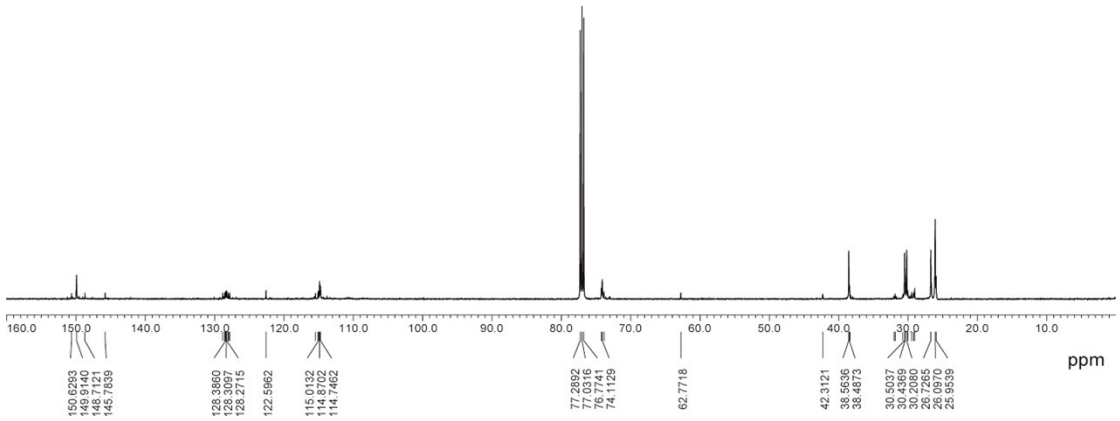


Fig. S2 ^{13}C NMR spectrum of **1d** in $CDCl_3$ at 25 °C.

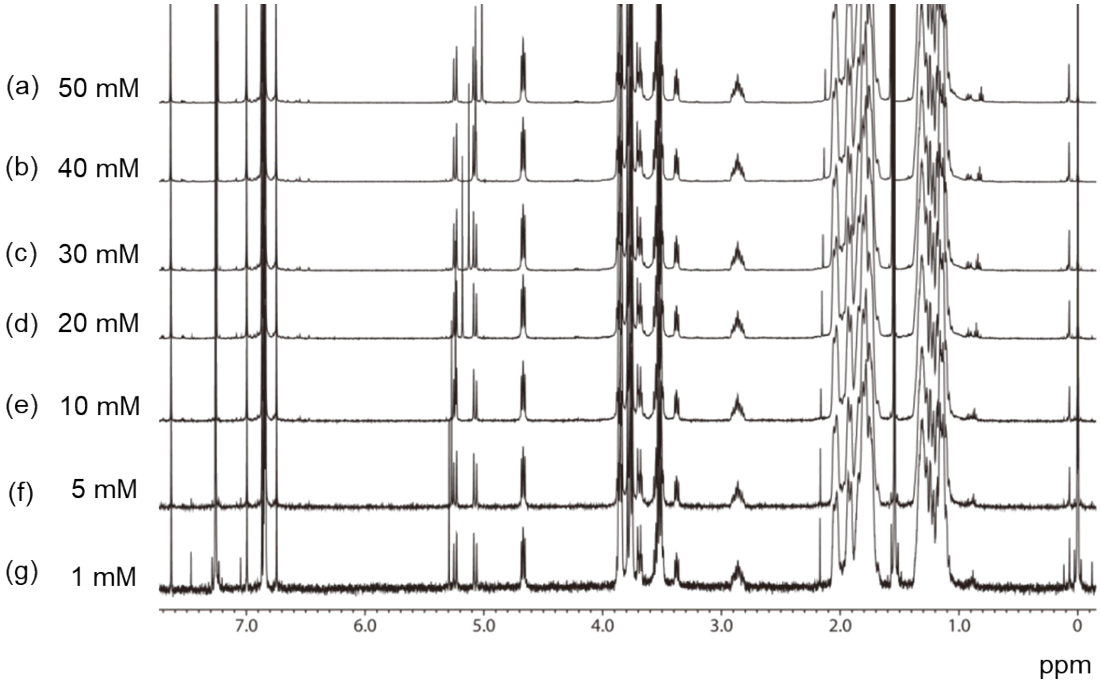
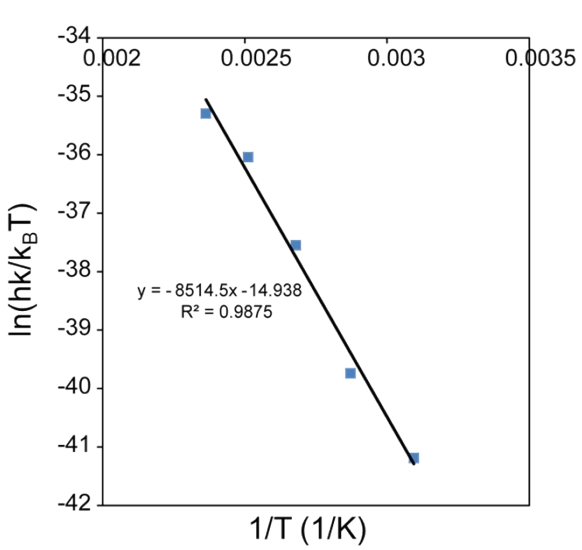


Fig. S3 ^{1}H NMR spectra of **1d** in various concentrations in $CDCl_3$.



$$\ln\left(\frac{hk}{k_B T}\right) = \frac{-\Delta G^{\ddagger}}{RT} \quad 、 \quad k = \frac{\ln 2}{t_{\frac{1}{2}}}$$

$$\Delta G^{\ddagger} = \Delta H^{\ddagger} - T\Delta S^{\ddagger}$$

$t_{1/2}$: Half-Life Time

$\Delta G^{\ddagger}$: Activation Free Energy

$$\Rightarrow \ln\left(\frac{hk}{k_B T}\right) = \frac{-\Delta H^{\ddagger}}{R}\frac{1}{T} + \frac{\Delta S^{\ddagger}}{R}$$

$\Delta H^{\ddagger}$ = 70.8 (kJ/mol)

$\Delta S^{\ddagger}$ = -124.2 (J/mol・K)

Fig. S4 Eyring plots in solid state self-incluson complexation.

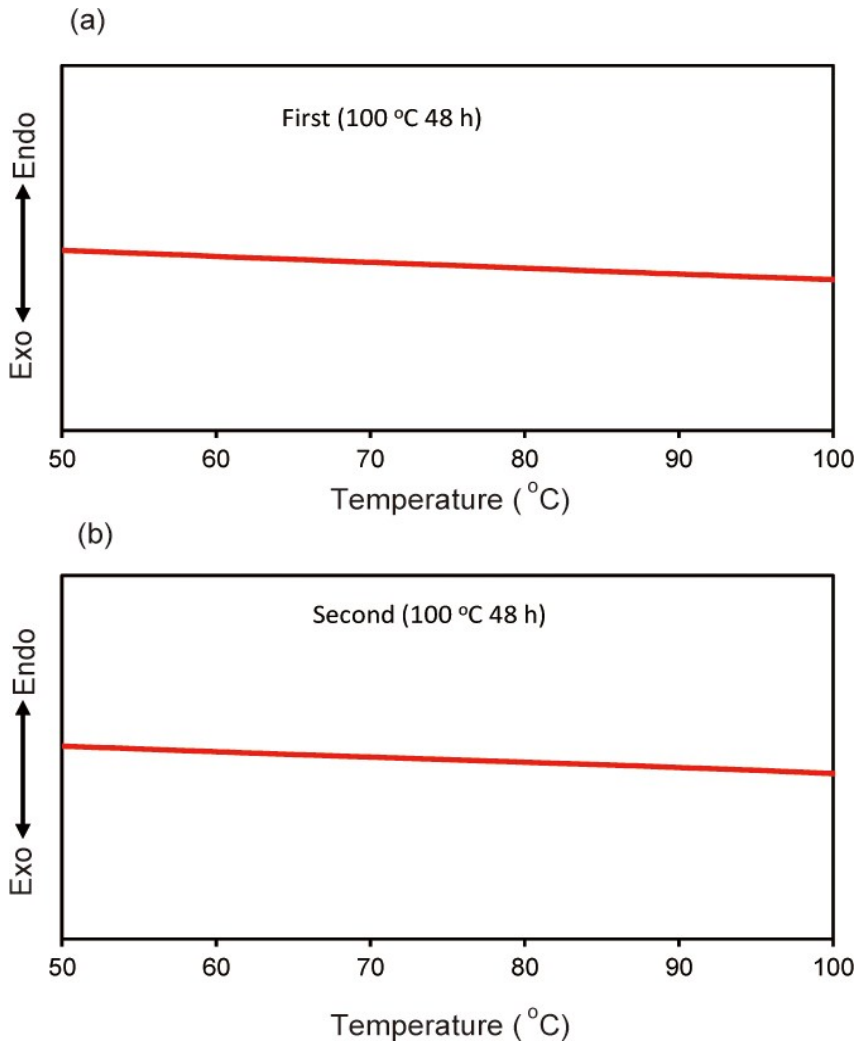


Fig. S5 DSC heating curves of a mixture of **1s** and **1d** (**1s**/**1d** = 85/15) in (a) first and (b) second heating processes. Therefore, the endothermic peak observed in the first heating of **1d** (**Fig. 3c**) resulted from formation of **1s**.

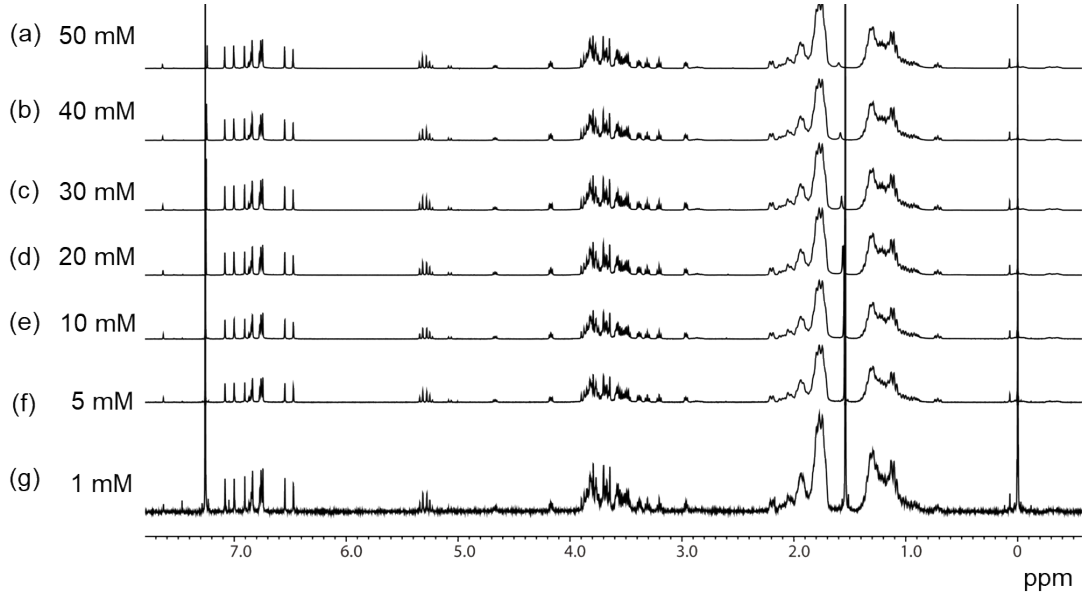


Fig. S6 ^{1}H NMR spectra of a mixture of **1s** and **1d** (**1s**/**1d** = 85/15) in various concentrations in $CDCl_3$.

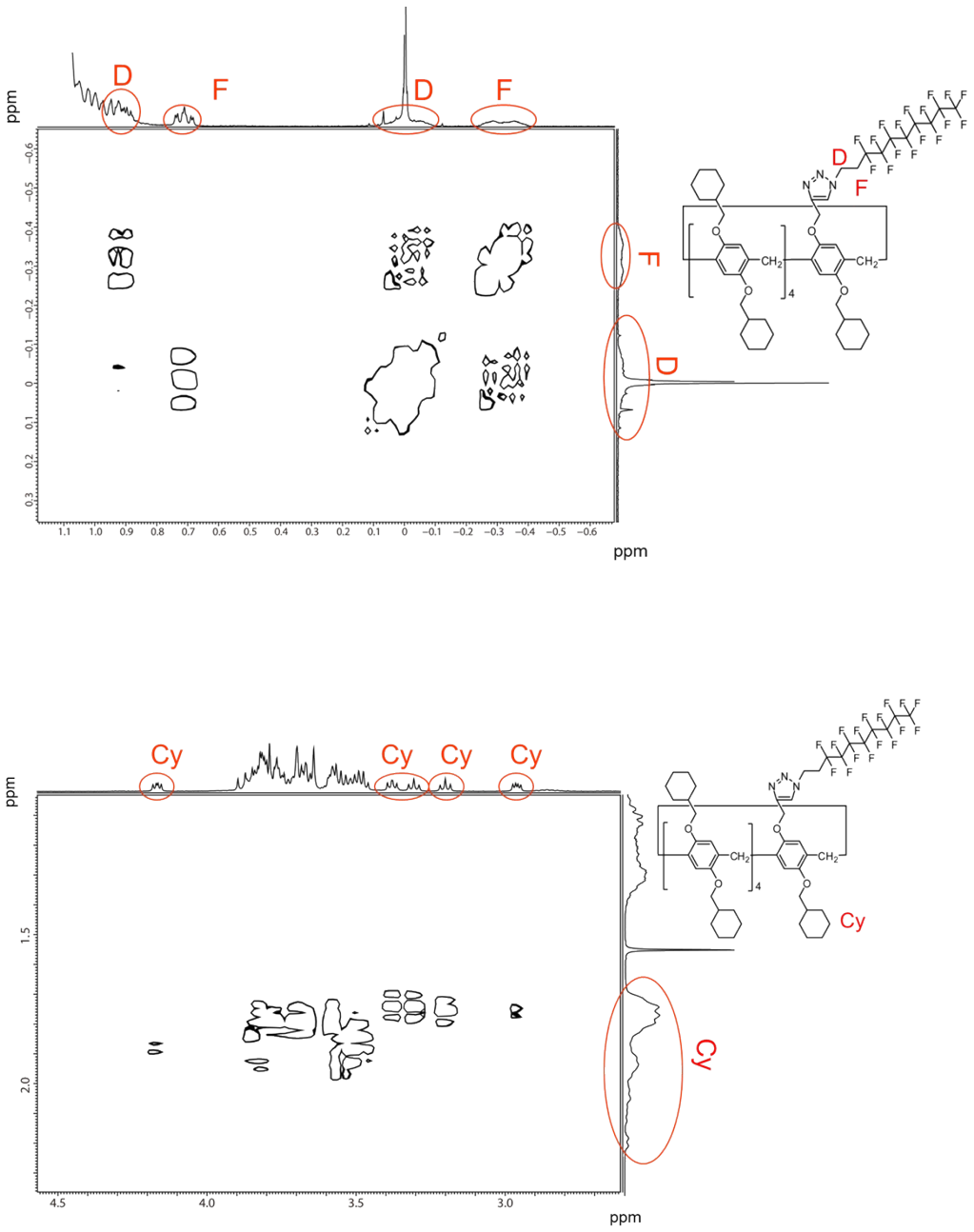


Fig. S7 COSY study of a mixture of **1s** and **1d** (**1s**/**1d** = 85/15) in $CDCl_3$.

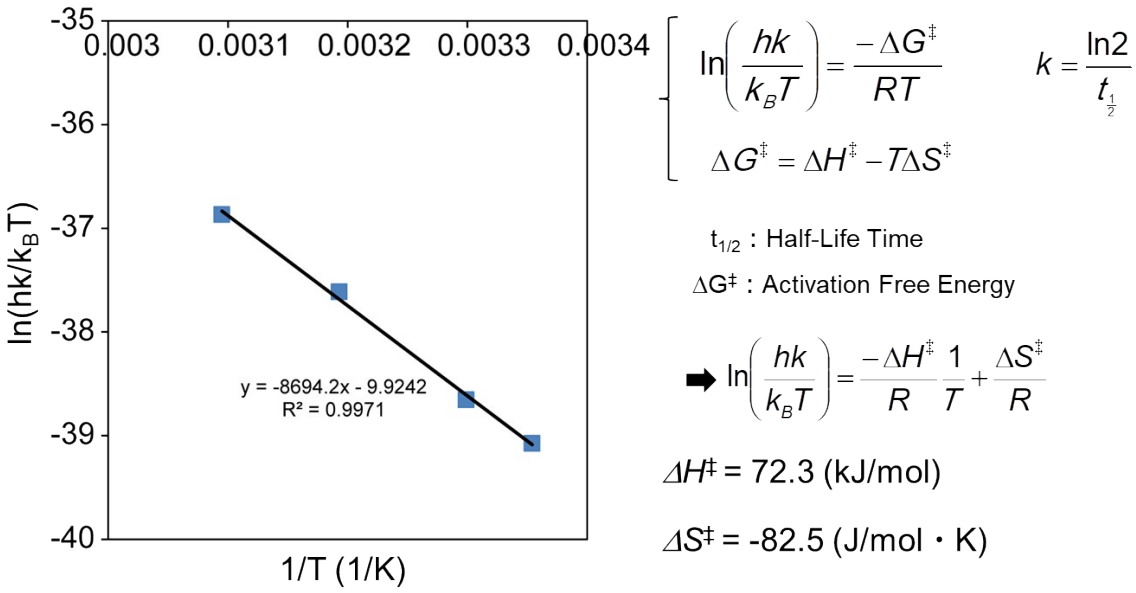


Fig. S8 Eyring plots in de-threading process in $CDCl_3$.

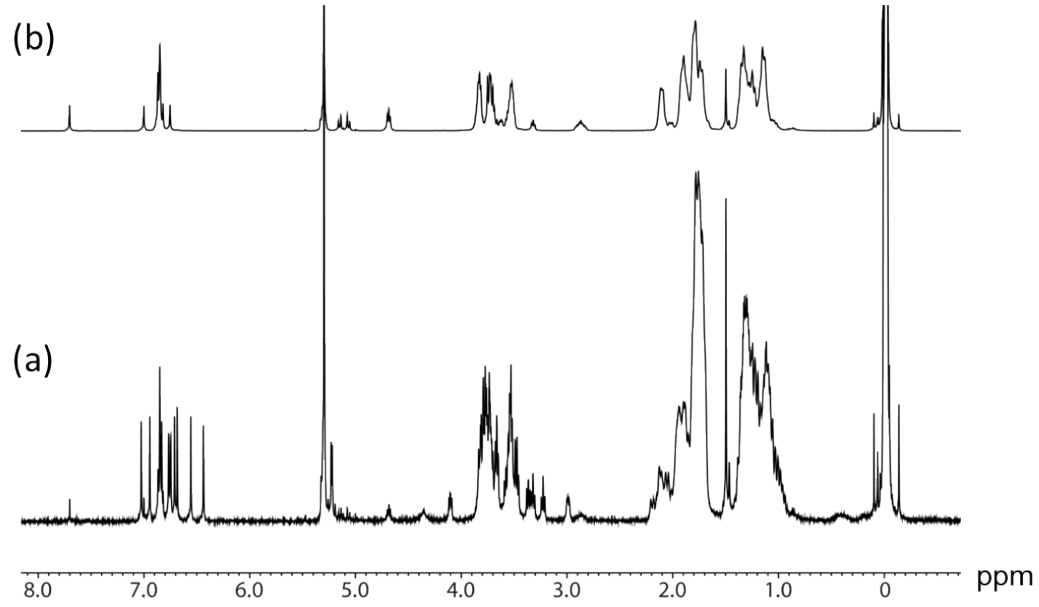


Fig. S9 ^{1}H NMR spectra after heating of **1** in the solid state at 100 °C for 48 h, dissolving the solid sample in CD_2Cl_2 and obtaining the spectrum after (a) 3 min and (b) 24 h. The spectra changed by storing a mixture of **1s** and **1d** (**1s**/**1d** = 85/15) in CD_2Cl_2 at 25 °C, indicationg that **1s** was slowly converted to **1d** in CD_2Cl_2.

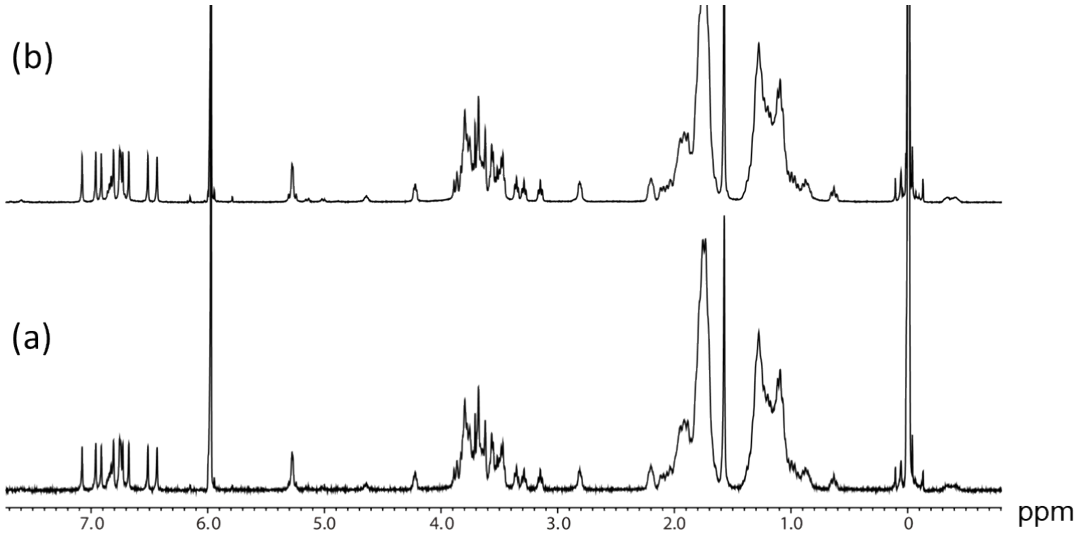


Fig. S10 ^{1}H NMR spectra after heating of **1** in the solid state at 100 ^{o}C for 48 h, dissolving the solid sample in deuterated 1,1,2,2-tetrachloroethane and obtaining the spectrum after (a) 3 min and (b) 24 h. The spectra did not change by storing a mixture of **1s** and **1d** (**1s**/**1d** = 85/15) in deuterated 1,1,2,2-tetrachloroethane at 25 ^{o}C, indicationg that **1s** was not converted to **1d** in deuterated 1,1,2,2-tetrachloroethane.

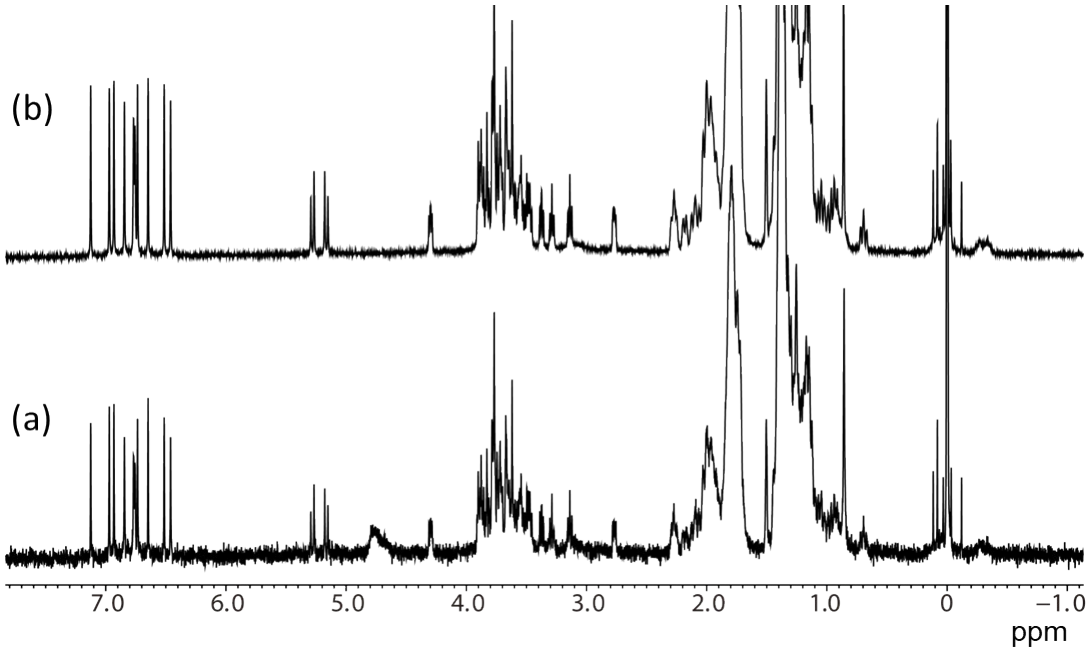


Fig. S11 ^{1}H NMR spectra after heating of **1** in the solid state at 100 ^{o}C for 48 h, dissolving the solid sample in deuterated cyclohexane and obtaining the spectrum after (a) 3 min and (b) 24 h. The spectra did not change by storing a mixture of **1s** and **1d** (**1s**/**1d** = 85/15) in deuterated cyclohexane at 25 ^{o}C, indicationg that **1s** was not converted to **1d** in deuterated cyclohexane.

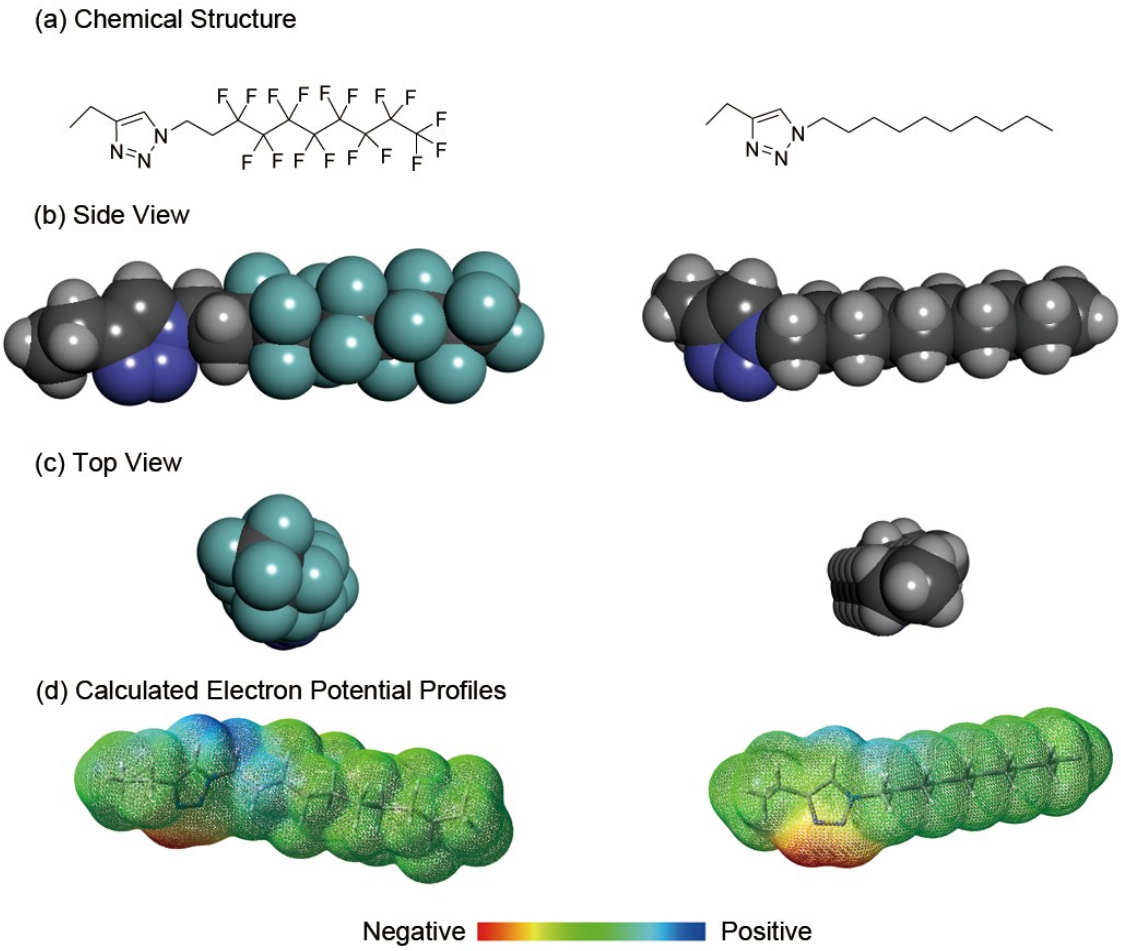


Fig. S12 (a) Chemical structures, (b,c) optimized structures and (d) calculated electron potential profiles (DFT calculations, B3LYP/6-31G(d,p)) of the guest part of **1** and alkyl chains as a reference.