Electronic Supplementary Information


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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$_3$.

**Fig. S4** Eyring plots in solid state self-inclusion complexation.

\[
\ln\left(\frac{hk}{k_B T}\right) = -\frac{\Delta G^\ddagger}{RT} \quad \text{and} \quad k = \ln\frac{2}{t_{1/2}}
\]

\[
\Delta G^\ddagger = \Delta H^\ddagger - T\Delta S^\ddagger
\]

$\Delta H^\ddagger$ : Activation Free Energy

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

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

$\Delta S^\ddagger = -124.2$ (J/mol · K)
Fig. 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 CDCl₃.
Fig. S8 Eyring plots in de-threading process in CDCl$_3$.

\[ \ln\left(\frac{h k}{k_B T}\right) = \frac{-\Delta G^\ddagger}{RT} \quad k = \frac{\ln 2}{t_{\frac{1}{2}}} \]
\[ \Delta G^\ddagger = \Delta H^\ddagger - T\Delta S^\ddagger \]
\[ t_{\frac{1}{2}} : \text{Half-Life Time} \]
\[ \Delta G^\ddagger : \text{Activation Free Energy} \]
\[ \ln\left(\frac{h k}{k_B T}\right) = \frac{-\Delta H^\ddagger}{R} \frac{1}{T} + \frac{\Delta S^\ddagger}{R} \]
\[ \Delta H^\ddagger = 72.3 \text{ (kJ/mol)} \]
\[ \Delta S^\ddagger = -82.5 \text{ (J/mol} \cdot \text{K)} \]

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$_2$Cl$_2$ 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$_2$Cl$_2$ at 25 °C, indicating that 1s was slowly converted to 1d in CD$_2$Cl$_2$. 
**Fig. S10** $^1$H NMR spectra after heating of 1 in the solid state at 100 °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 °C, indicating 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 °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 °C, indicating 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.