Electronic Supplementary Information

A stable *cis*-stilbene derivative encapsulated in cucurbit[7]uril

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Determination of binding constants

The binding constants were determined by UV titration on a Hewlett-Packard 8453 diode array spectrophotometer. The experiments were carried out in 2 M citric acid / sodium hydroxide buffer solution (pH 3). The guest (*trans*-**1**, *cis*-**1**) concentration ($[\mathbf{1}^0]$) was held constant (6×10^{-5} M) and the CB[7] concentration ($[\mathrm{CB[7]}^0]$) was varied ($0 - 2.4 \times 10^{-4}$ M). The concentration of *trans*-**1** was calculated by using molar absorption coefficient at 296 nm ($\varepsilon_{trans\text{-}\mathbf{1}} = 25800\ \mathrm{M^{-1}cm^{-1}}$).[1] From this data, the molar absorption coefficients of *cis*-**1**, *trans*-**1**$\subset$CB[7] and *cis*-**1**$\subset$CB[7] were estimated to be 9100 $\mathrm{M^{-1}cm^{-1}}$, 20800 $\mathrm{M^{-1}cm^{-1}}$, 7900 $\mathrm{M^{-1}cm^{-1}}$ respectively. Fig. S1 shows the gradual change in UV-vis absorption spectra of *trans*-**1** and *cis*-**1** with the addition of 0-4 equivalents of CB[7]. The effect of molar ratio $[\mathbf{1}^0] / [\mathrm{CB[7]}^0]$ change on the absorbance of **1** at 296 nm is shown on Fig. S2.

The stability constants were calculated by using modified Rose-Drago equation:[2] The Rose-Drago expression for the stability constant $K = [\mathbf{1}\subset\mathrm{CB[7]}] / [\mathbf{1}] \times [\mathrm{CB[7]}]$, for the reaction $\mathbf{1} + \mathrm{CB[7]} = \mathbf{1}\subset\mathrm{CB[7]}$, where $[\mathbf{1}]$, $[\mathrm{CB[7]}]$ and $[\mathbf{1}\subset\mathrm{CB[7]}]$ represent equilibrium concentration of **1**, CB[7] and **1**$\subset$CB[7], respectively, is:

$$([\mathbf{1}^0] + [\mathrm{CB[7]}^0]) / \Delta\varepsilon_{\mathbf{1}\subset\mathrm{CB[7]}} + 1 / (K \times \Delta\varepsilon_{\mathbf{1}\subset\mathrm{CB[7]}}) = ([\mathbf{1}^0] \times [\mathrm{CB[7]}^0] / \Delta A) + \Delta A / \Delta\varepsilon^2_{\mathbf{1}\subset\mathrm{CB[7]}} \tag{1}$$

in which, $\Delta\varepsilon_{\mathbf{1}\subset\mathrm{CB[7]}} = \varepsilon_{\mathbf{1}} - \varepsilon_{\mathbf{1}\subset\mathrm{CB[7]}}$, where $\varepsilon_{\mathbf{1}}$, $\varepsilon_{\mathbf{1}\subset\mathrm{CB[7]}}$ represent the molar absorption coefficients of **1** and **1**$\subset$CB[7], respectively; $\Delta A = A - A_0$, A_0 is the initial solution absorbance at 296 nm in absence of CB[7] and A is the observed solution absorbance in the presence of CB[7].

According to Equation (1) a plot of $([\mathbf{1}^0] \times [\mathrm{CB[7]}^0] / \Delta A) + \Delta A / \Delta\varepsilon^2_{\mathbf{1}\subset\mathrm{CB[7]}}$ versus $[\mathbf{1}^0] + [\mathrm{CB[7]}^0]$ gives a straight line with an intercept of $1 / (K \times \Delta\varepsilon_{\mathbf{1}\subset\mathrm{CB[7]}})$, from which the constants were calculated (Fig. S3).

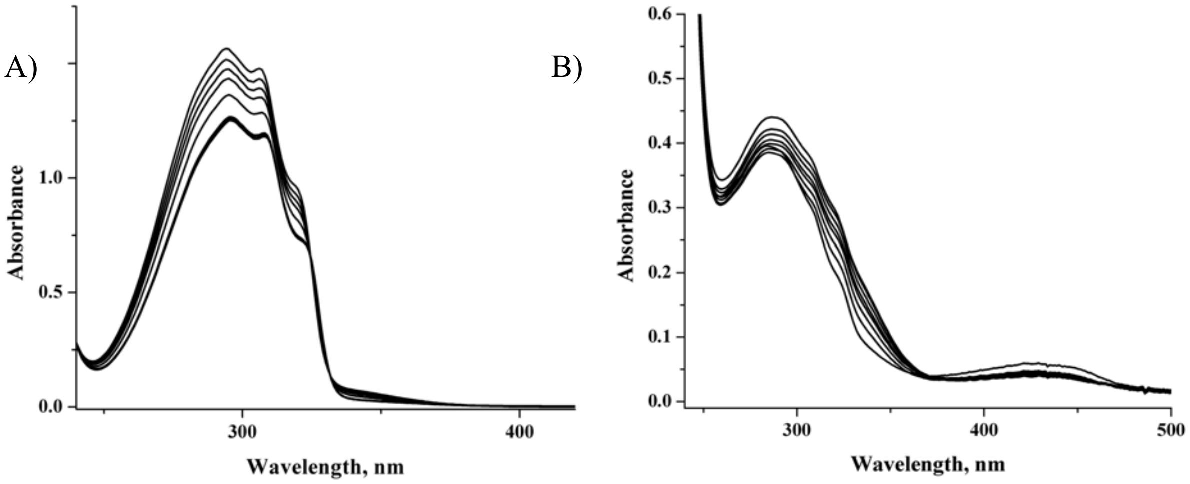

Fig. S1 UV spectral change during addition of CB[7] to (A) *trans*-**1** solution, and (B) *cis*-**1** solution.

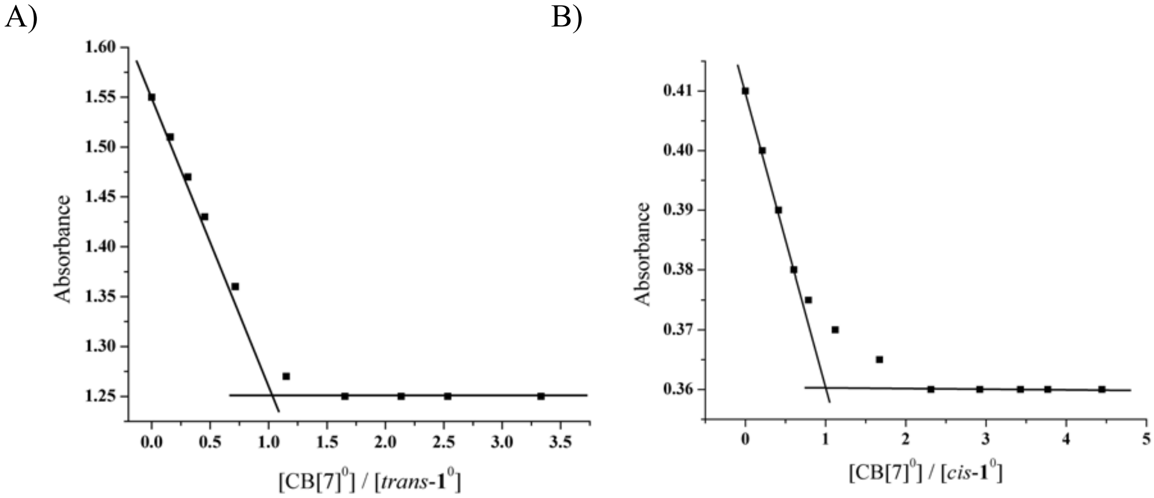

Fig. S2 The effect of molar ratio [CB[7]^0] / [**1**^{0}] change on the absorbance of (A) *trans*-**1**, and (B) *cis*-**1**, at λ_{max} 296 nm. The plots also show that the complexes are formed in a 1:1 molar ratio.

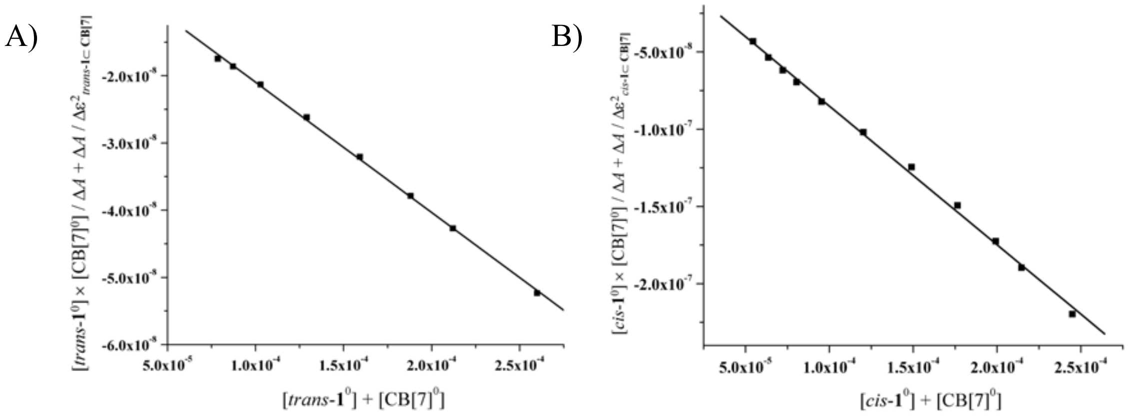

Fig. S3 Plots of Equation (1) for 1:1 complexation of CB[7] with (A) *trans*-**1**, and (B) *cis*-**1**.

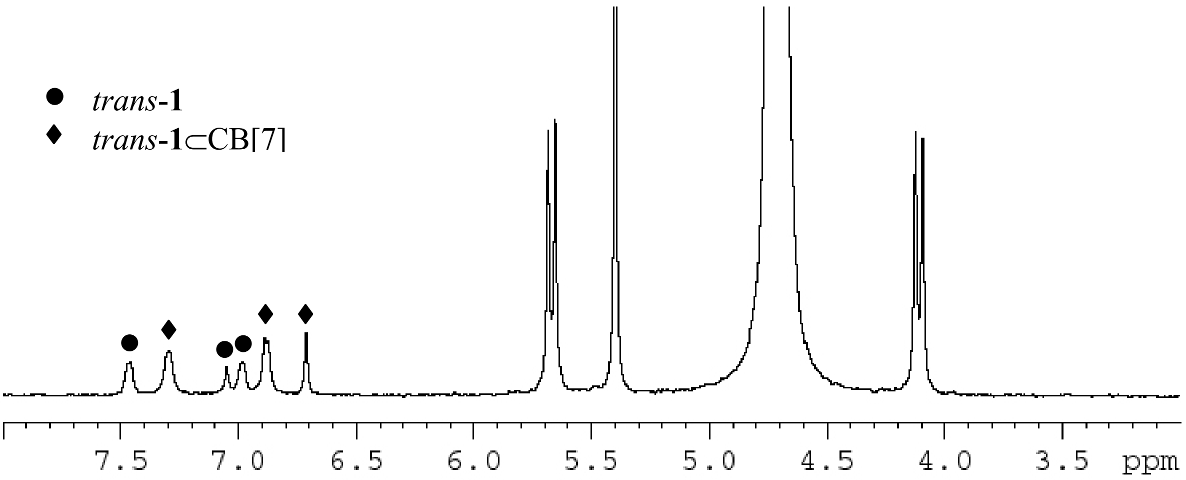

Fig. S4 ^{1}H NMR spectrum of *trans*-**1** in the presence of 0.6 equivalent CB[7] showing two sets of signals, one for free *trans*-**1** and the other for *trans*-**1**$\subset$CB[7].

References

1 Y. Zhao, V. Khodorkovsky, J. Cohen and Z. Priel, *J. Photochem. Photobiol., A*, 1996, **99**, 23.

2 M. Nishida, D. Ishii, I. Yoshida and S. Shinkai, *Bull. Chem. Soc. Jpn.,* 1997, **70**, 2131.