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On the thermodynamic and kinetic investigations of a [*c*2]daisy chain polymer

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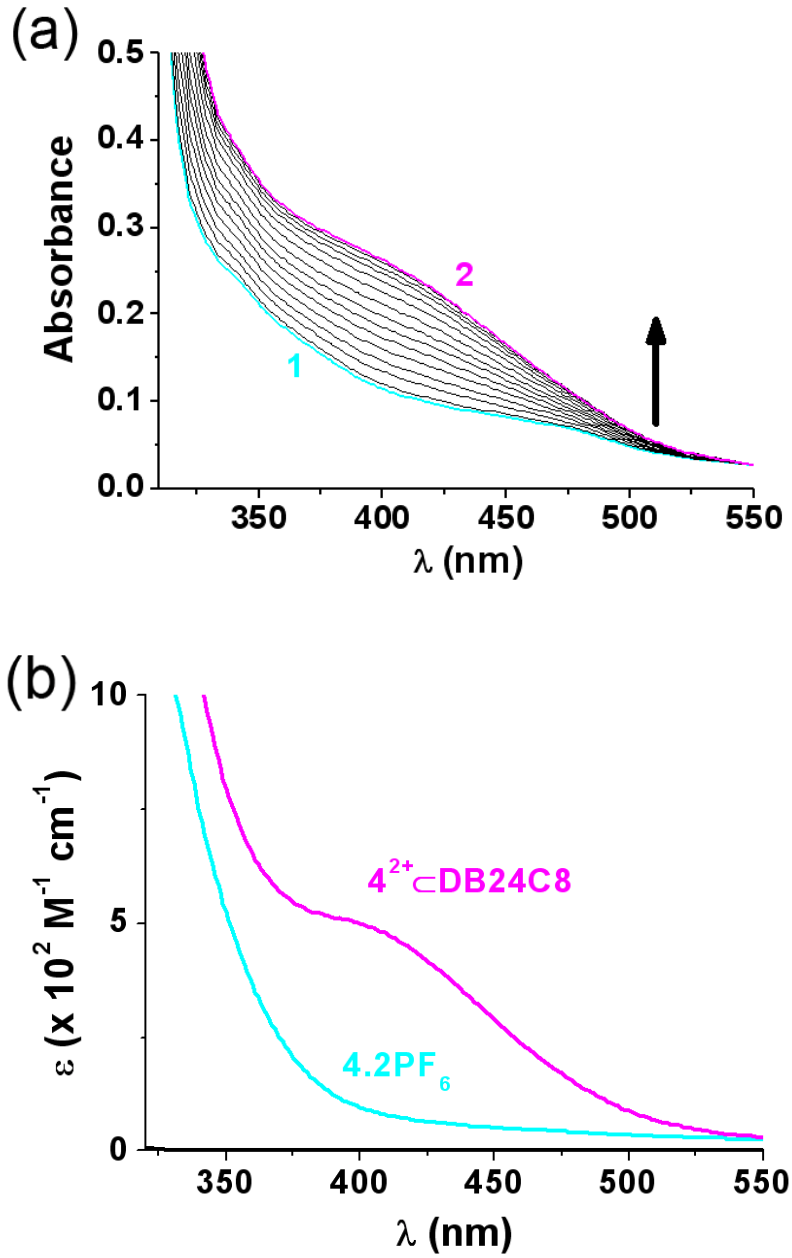

Figure S1: (a) UV-Visible absorption spectrophotometric titration of **4**·2PF_6 with **DB24C8**. [**4**·2PF_6]$_{tot}$ = 1.44 × 10^{-3} M; (**1**) [**DB24C8**]$_{tot}$ / [**4**·2PF_6]$_{tot}$ = 0; (**2**) [**DB24C8**]$_{tot}$ / [**4**·2PF_6]$_{tot}$ = 12.8; l = 1 cm. (b) Absorption electronic spectra of **4**·2PF_6 substrate and of **4^{2+}⊂DB24C8** complex. Solvent: MeCN; T = 25.0(2) °C.

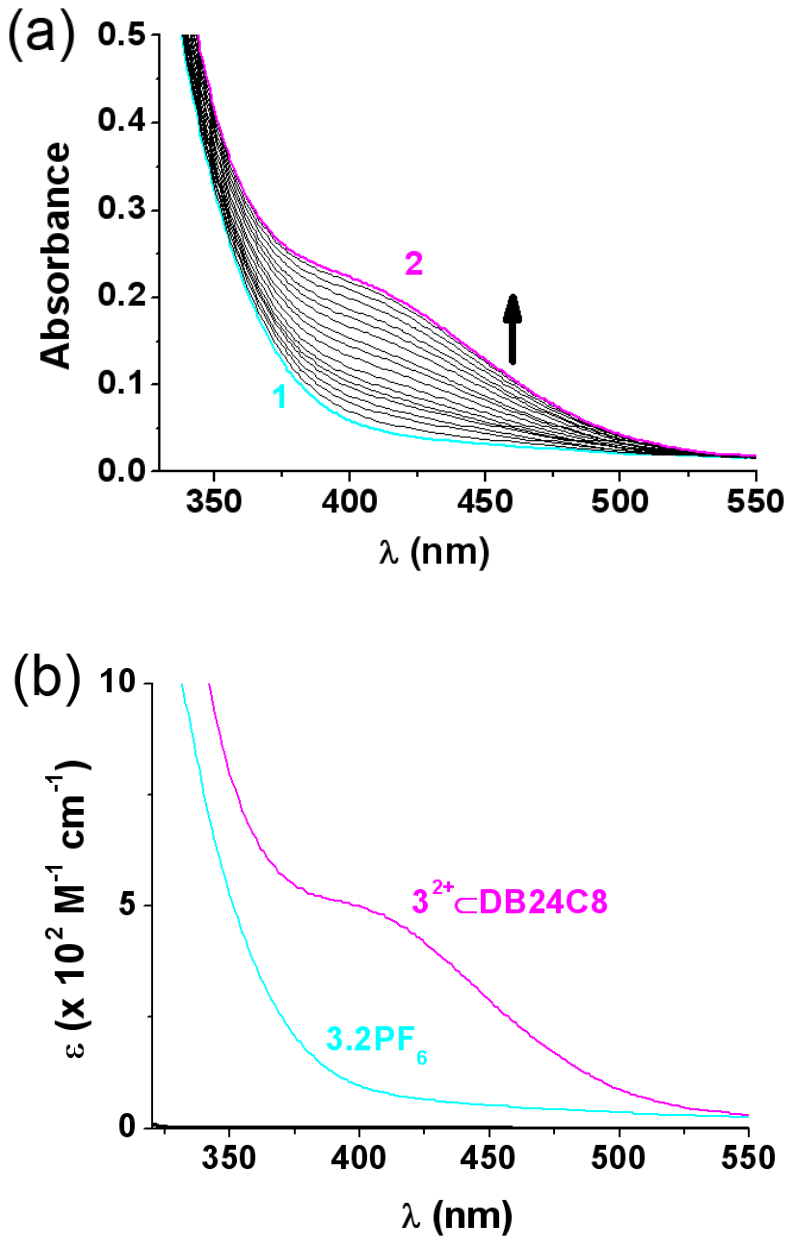

Figure S2: (a) UV-Visible absorption spectrophotometric titration of **3**·2PF_6 with **DB24C8**. [**3**·2PF_6]$_{tot}$ = 6.14 × 10^{-4} M; (**1**) [**DB24C8**]$_{tot}$ / [**3**·2PF_6]$_{tot}$ = 0; (**2**) [**DB24C8**]$_{tot}$ / [**3**·2PF_6]$_{tot}$ = 35.8; l = 1 cm. (b) Absorption electronic spectra of **3**·2PF_6 substrate and of **3^{2+}⊂DB24C8** complex. Solvent: MeCN; T = 25.0(2) °C.

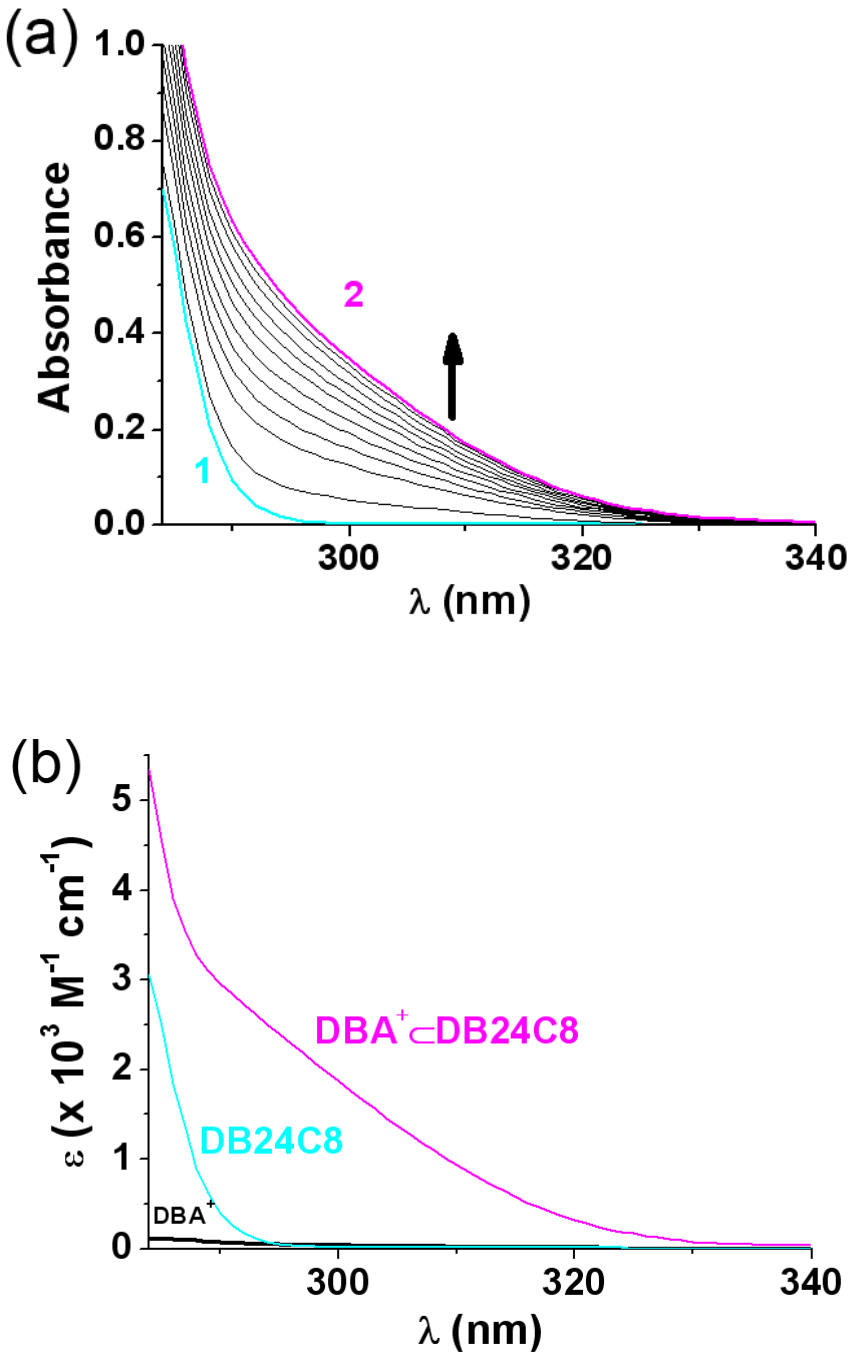

Figure S3: (a) UV-Visible absorption spectrophotometric titration of **DB24C8** with **DBA**·CF_3CO_2. $[\mathbf{DB24C8}]_{tot} = 1.128 \times 10^{-3}$ M; (**1**) $[\mathbf{DBA}\cdot CF_3CO_2]_{tot}$ / $[\mathbf{DB24C8}]_{tot} = 0$; (**2**) $[\mathbf{DBA}\cdot CF_3CO_2]_{tot}$ / $[\mathbf{DB24C8}]_{tot} = 12.2$; $l = 0.2$ cm. (b) Absorption electronic spectra of **DBA**·CF_3CO_2 substrate, of DB24C8 receptor and of $\mathbf{DBA}^+\subset\mathbf{DB24C8}$ complex. Solvent: MeCN; $T = 25.0(2)$ °C.

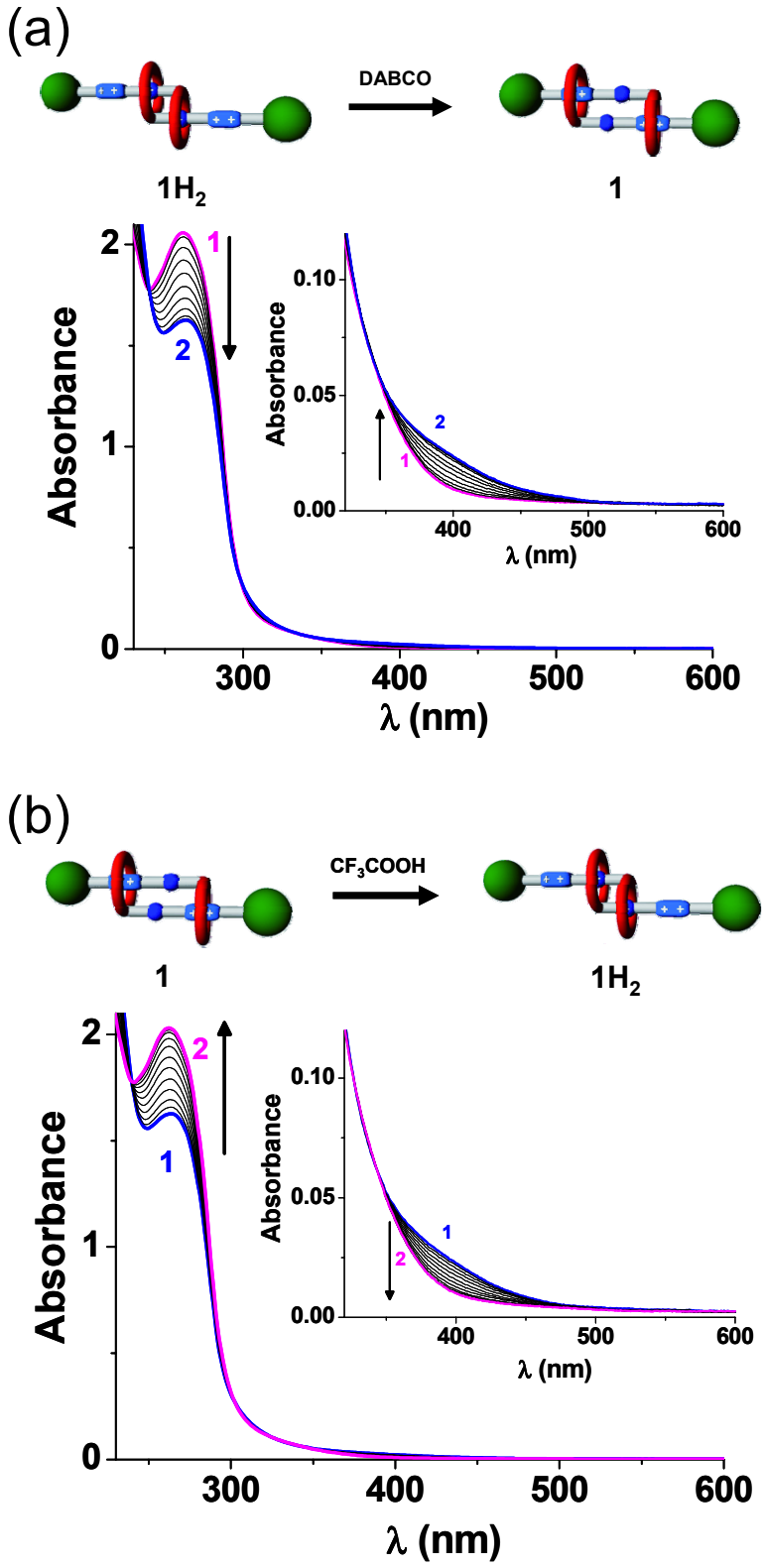

Figure S4. UV-Vis absorption spectrophotometric variations recorded in MeCN upon addition of (a) DABCO to a solution of $\mathbf{1}H_2{\cdot}6PF_6$ and $[\mathbf{1}H_2{\cdot}6PF_6]_{tot} = 4.08 \times 10^{-5}$ M; (1) $[DABCO]_{tot} / [\mathbf{1}H_2{\cdot}6PF_6]_{tot} = 0$; (2) $[DABCO]_{tot} / [\mathbf{1}H_2{\cdot}6PF_6]_{tot} = 4.0$. (b) CF_3CO_2H to a solution of $(\mathbf{1}{\cdot}4PF_6)$. Solvent: MeCN; T = 25.0(2) °C; l = 1 cm.

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$[(\mathbf{1}\cdot 4PF_6)]_{tot} = 4.08 \times 10^{-5}$ M; (1) $[CF_3CO_2H]_{tot} / [(\mathbf{1}\cdot 4PF_6)]_{tot} = 0$; (2) $[CF_3CO_2H]_{tot} / [(\mathbf{1}\cdot 4PF6)]_{tot} = 5.8$

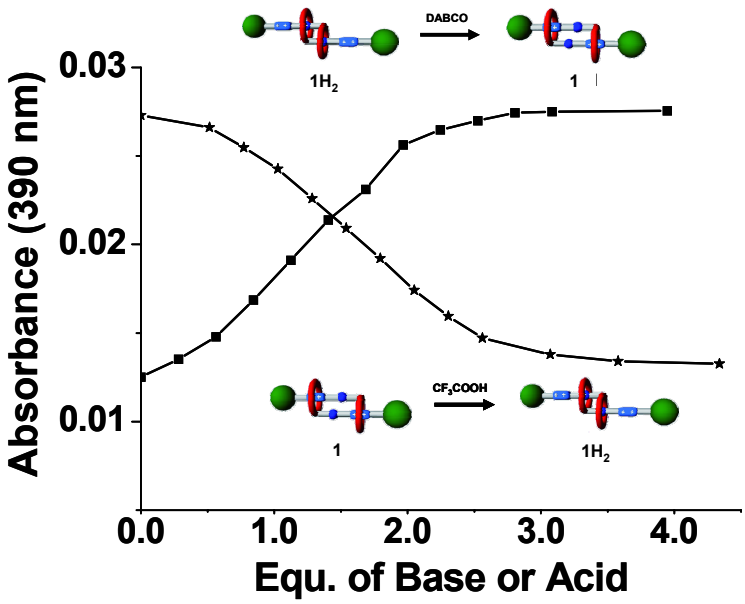

Figure S5. Variation in the absorbance of the CT band (λ= 390 nm) with the gradual addition of DABCO or CF_3CO_2H to monomer $\mathbf{1}H_2 \cdot 6PF_6$. Solvent: MeCN; T = 25.0(2) °C; l = 1 cm; $[\mathbf{1}H_2 \cdot 6PF_6]_{tot} = [1 \cdot 4PF_6]_{tot} = 4.08 \times 10^{-5}$ M.

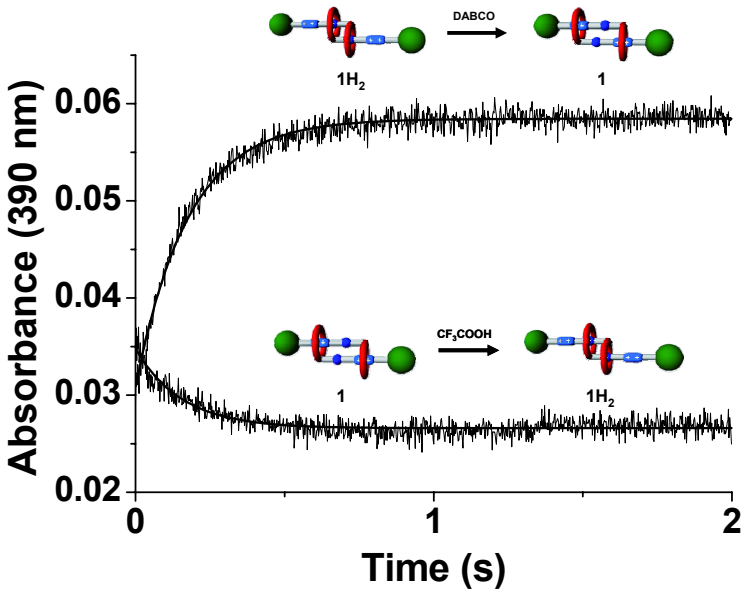

Figure S6. Variation of the absorbance at λ = 390 nm (CT absorption) versus time for the acid-induced extension and the base-promoted contraction of the [*c*2] daisy chain monomer $\mathbf{1}H_2 \cdot 6PF_6$. Solvent: MeCN; T = 25.0(2) °C; l = 1 cm; $[\mathbf{1}H_2 \cdot 6PF_6]_{tot} = 7.27 \times 10^{-5}$ M; $[DABCO]_{tot} = 2.56 \times 10^{-3}$ M; $[\mathbf{1} \cdot 4PF_6]_{tot} = 7.05 \times 10^{-5}$ M; $[CF_3CO_2H]_{tot} = 2.93 \times 10^{-3}$ M.

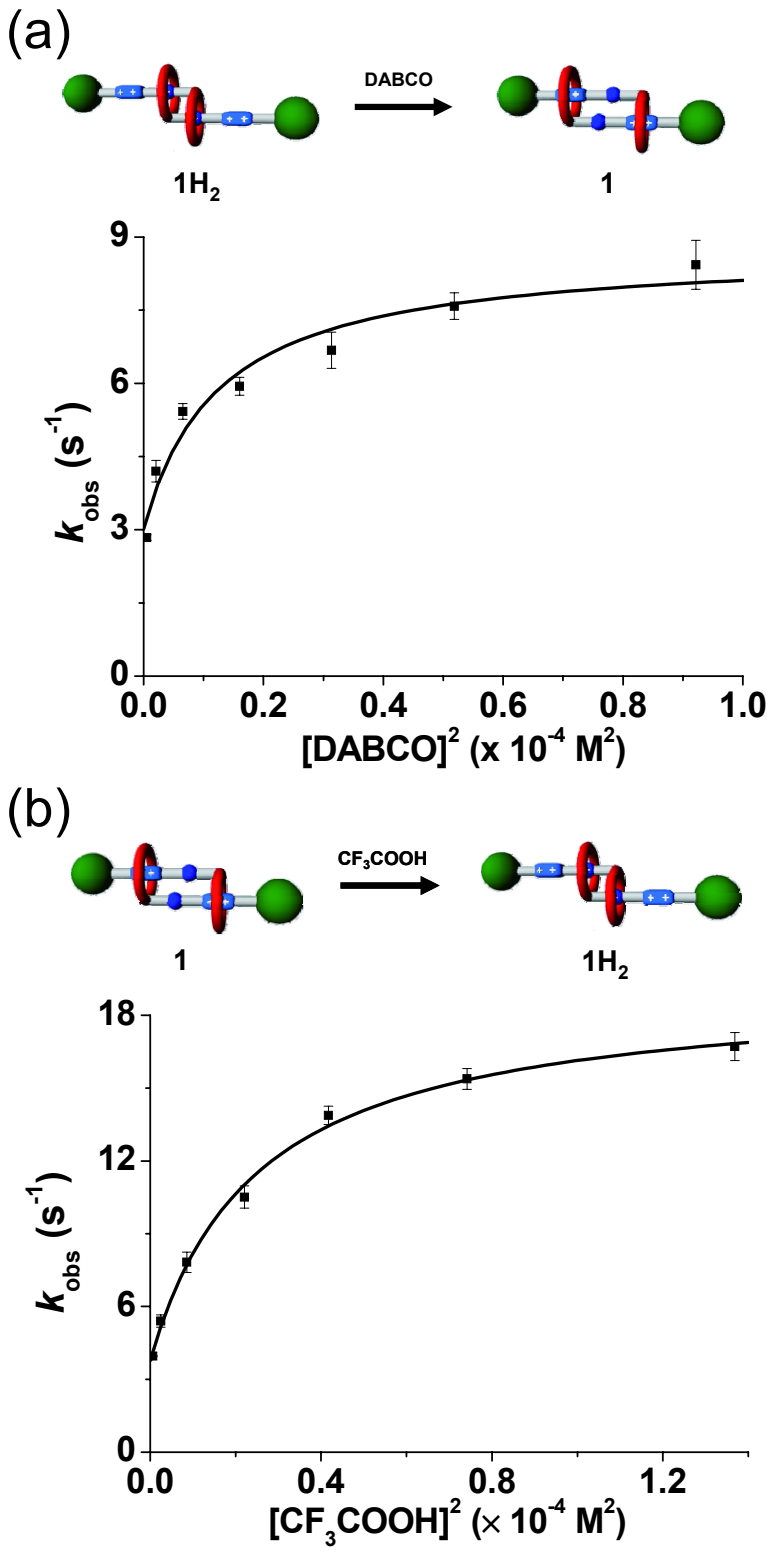

Figure S7. Variations of the pseudo-first-order rate constants k_{obs} (s^{-1}), relative to the base-induced contraction (a) and acid-triggered extension (b) of the [*c*2]daisy chain monomer as a function of $[DABCO]_{tot}$ and $[CF_3CO_2H]_{tot}$, respectively. Solvent: acetonitrile; T = 25.0(2) °C. (a) $[\mathbf{1}H_2{\cdot}6PF_6]_{tot} = 7.27 \times 10^{-5}$ M; (b) $[\mathbf{1}{\cdot}4PF_6]_{tot} = 7.05 \times 10^{-5}$ M.

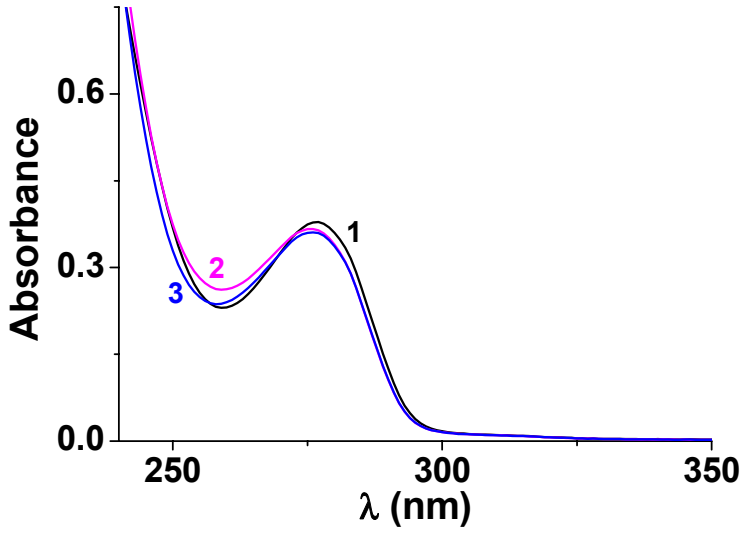

Figure S8. Spectral changes observed on addition of DABCO to a solution of the dimeric self-complex (**5**H·PF_6)$_2$. Solvent: MeCN; T = 25.0(2) °C; l = 0.2 cm; [(**5**H·PF_6)$_2$]$_{tot}$ =2.25 × 10^{-4} M; (**1**) [DABCO] / [(**5**H·PF_6)$_2$] = 0; (**2**) [DABCO] / [(**5**H·PF_6)$_2$] = 8 (immediately recorded after addition of DABCO); (**3**) [DABCO] / [(**5**H·PF_6)$_2$] = 8 (recorded after 10 minutes).

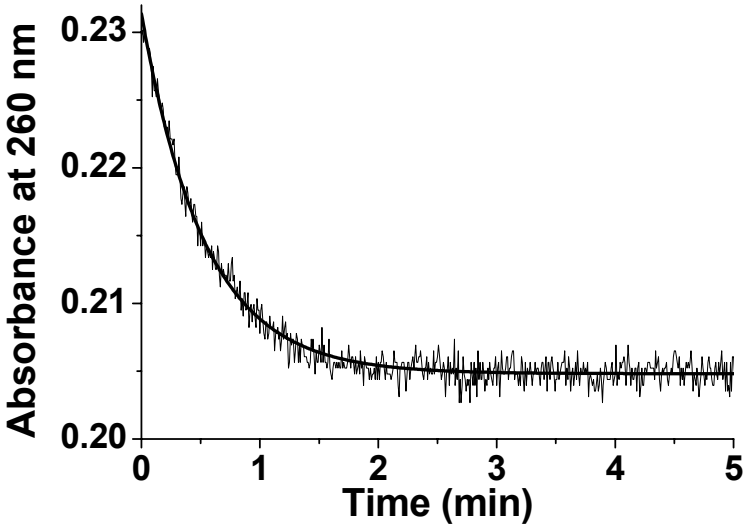

Figure S9. Variation of the absorbance at λ = 260 nm versus time for the base-induced dissociation of the dimeric self-complex (**5**H·PF_6)$_2$. Solvent: MeCN; T = 25.0(2) °C; l = 0.2 cm; [(**5**H·PF_6)$_2$]$_{tot}$ = 2.15 × 10^{-4} M; [DABCO]$_{tot}$ = 4.42 × 10^{-3} M.

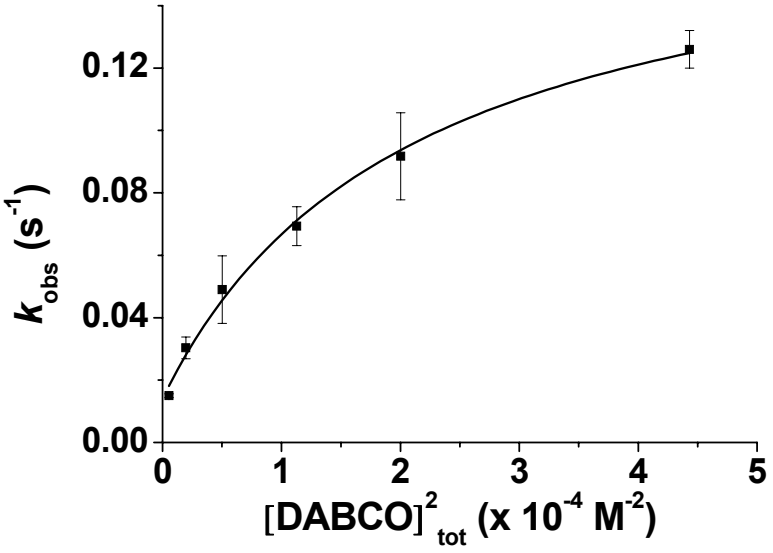

Figure S10. Variations of the pseudo-first-order rate constants k_{obs} (s^{-1}) relative to the base-induced dissociation of the dimeric self-complex (**5**H·PF_6)$_2$ as a function of $[DABCO]_{tot}$. Solvent: MeCN; T = 25.0(2) °C; l = 0.2 cm; $[(\mathbf{5}H\cdot PF_6)_2]_{tot}$ = 2.15 × 10^{-4} M.