Relative Unidirectional Translation in an Artificial Molecular Assembly Fueled by Light

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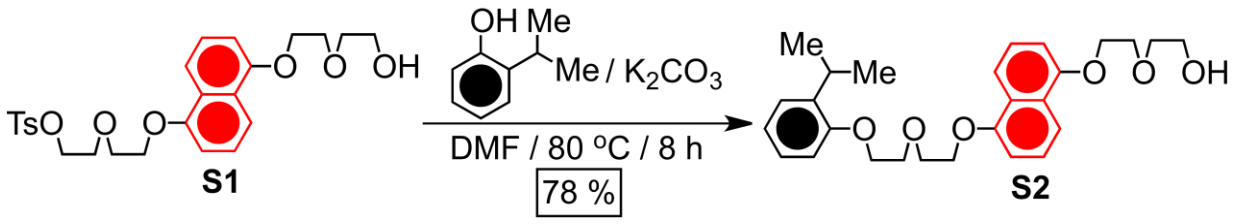
Supporting Information

1. General Methods

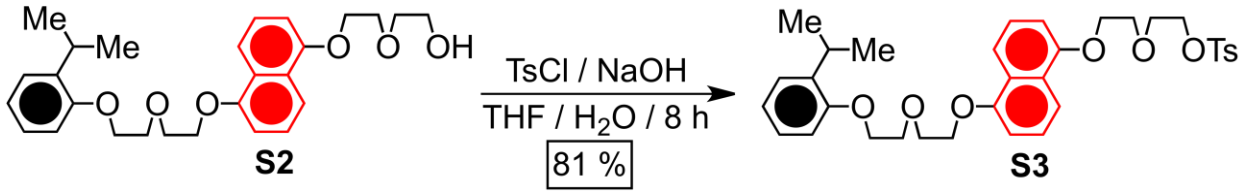
All reagents were purchased from commercial suppliers (Aldrich or Fisher) and used without further purification. Cyclobis(paraquat-*p*-phenylene) hexafluorophosphate [S1] (**CBPQT**·$4PF_6$), and compounds **S1**[S2], **2**[S3], **3**[S4], as well as the [2]rotaxane **R1**·$4PF_6$[S5] were all prepared according to literature procedures. Thin layer chromatography (TLC) was performed on silica gel 60 F254 (E. Merck). Column chromatography was carried out on silica gel 60F (Merck 9385, 0.040–0.063 mm). UV/Vis spectra were recorded on a Varian 100-Bio UV-Vis spectrophotometer in MeCN at room temperature. Nuclear magnetic resonance (NMR) spectra were recorded on Bruker Avance 600 or Varian P-Inova 500 spectrometers, with working frequencies of 600 and 500 MHz for ^1H, and 150 and 125 MHz for ^{13}C nuclei, respectively. Chemical shifts are reported in ppm relative to the signals corresponding to the residual non-deuterated solvents ($CDCl_3$: δ = 7.26 ppm, CD_3CN: δ =1.94 ppm). High-resolution mass spectra were measured, either on an Applied Biosystems Voyager DE-PRO MALDI TOF mass spectrometer (HR-TOF), or on a Finnigan LCQ iontrap mass spectrometer (HR-ESI). Cyclic voltammetry (CV) experiments were carried out at room temperature in argon-purged solutions in MeCN with a Gamry Multipurpose instrument (Reference 600) interfaced to a PC. CV Experiments were performed using a glassy carbon working electrode (0.071 cm^2). The electrode surface was polished routinely with 0.05 μm alumina-water slurry on a felt surface immediately before use. The counter electrode was a Pt coil and the reference electrode was silver/silver chloride. The concentration of the sample and supporting electrolyte (tetrabutylammonium hexafluorophosphate or tetrabutylammonium chloride) were 1.0×10^{-3} mol L^{-1} and 0.1 mol L^{-1}, respectively. For the visible light lamp, we employed a standard incandescent bulb (60 W) without taking any extra precautions to select for specific wavelengths.

2. Synthetic Procedures



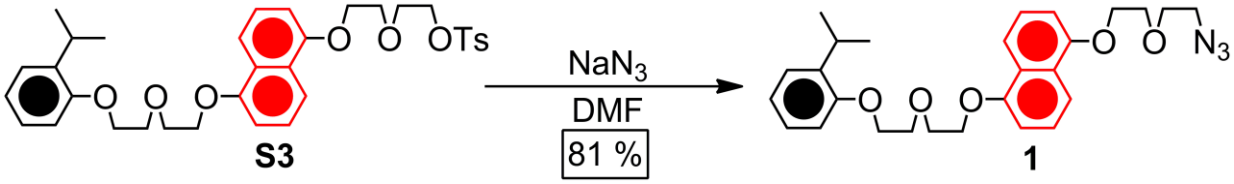
Scheme S1. Synthesis of **S2**

S2: Compound **S1** (490 mg, 1 mmol), 2-isopropylphenol (150 mg, 1.1 mmol) and K_2CO_3 (1.38 g, 10 mmol) were added to a round-bottomed flask (250 mL) containing dry DMF (50 mL). The reaction mixture was stirred at 80 °C for 8 h. After cooling to room temperature, the solution was poured into H_2O (200 mL). The resulting mixture was extracted with EtOAc (3 x 20 mL) and the combined organic phases were washed three times with saturated aqueous NaCl solution (3 x 100 mL). After drying ($MgSO_4$), the solvent was removed in vacuo and the resulting residue was purified by column chromatography (SiO_2: Hexanes / EtOAc 50:50) to afford the desired product **S2** (354 mg, 78%) as a light-yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.92 (d, J = 8.5 Hz, 1H), 7.90 (d, J = 8.5 Hz, 1H), 7.40 (t, J = 8.5 Hz, 1H), 7.37 (t, J = 8.5 Hz, 1H), 7.25 (dd, J = 7.5, 1.5 Hz, 1H), 7.17 (td, J = 8.0, 1.5 Hz, 1H), 6.99–6.96 (m, 1H), 6.89–6.86 (m, 3H), 4.35 (t, J = 5.0 Hz, 2H), 4.31 (t, J = 5.0 Hz, 2H), 4.21 (t, J = 5.0 Hz, 2H), 4.11 (t, J = 5.0 Hz, 2H), 4.06 (t, J = 5.0 Hz, 2H), 4.02 (t, J = 5.0 Hz, 2H), 3.80 (b, 2H), 3.76 (t, J = 5.0 Hz, 2H), 3.40 (septet, J = 7.0 Hz, 1H), 1.25 (d, J = 7.0 Hz, 6H). ^{13}C NMR (125 MHz, $CDCl_3$): δ = 156.0, 154.4, 154.2, 137.3, 126.8, 126.7, 126.6, 126.1, 125.3, 125.1, 120.9, 114.8, 114.5, 111.5, 105.8, 105.7, 72.7, 70.3, 70.0, 69.8, 68.0, 67.9, 67.8, 61.9, 26.9, 22.7. MS (MALDI–TOF) calcd for m/z = 454.235 $[M]^+$, found m/z = 454.344.



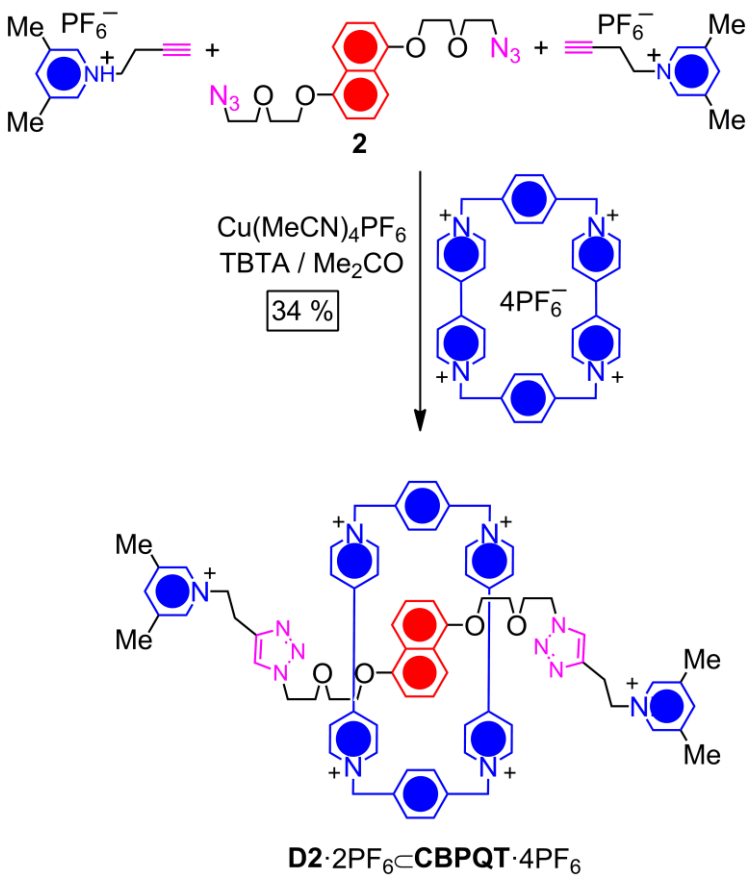
Scheme S2. Synthesis of **S3**

S3: A 50% aqueous NaOH solution (8 mL) was added to a solution of compound **S2** (227 mg, 0.5 mmol) in THF (50 mL) at 0 °C. After stirring the mixture for 30 min, TsCl (96 mg, 0.5 mmol) in THF (50 mL) was added slowly to the solution. The reaction mixture was stirred for 8 h, and then poured into H_2O. The resulting mixture was extracted with $CHCl_3$ (3 x 20 mL) and the combined organic phases were washed with a saturated aqueous NaCl solution (3 x 100 mL). After drying ($MgSO_4$), the solvent was removed under reduced pressure. The residue was purified by column chromatography (SiO_2: Hexanes / EtOAc 80:20) to afford the desired tosylate **S3** (246 mg, 81%) as a light-yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.89 (d, J = 8.5 Hz, 1H), 7.81 (d, J = 8.5 Hz, 1H), 7.78 (d, J = 8.5 Hz, 2H), 7.35 (t, J = 8.5 Hz, 1H), 7.33 (t, J = 8.5 Hz, 1H), 7.24–7.21 (m, 3H), 7.14 (td, J = 8.0, 1.5 Hz, 1H), 6.93 (td, J = 8.0, 1.5 Hz, 1H), 6.86 (d, J = 7.5 Hz, 1H), 6.85 (d, J = 7.5 Hz, 1H), 6.80 (d, J = 7.5 Hz, 1H), 4.32 (t, J = 5.0 Hz, 2H), 4.22 (t, J = 5.0 Hz, 2H), 4.21–4.18 (m, 4H), 4.09 (t, J = 5.0 Hz, 2H), 4.03 (t, J = 5.0 Hz, 2H), 3.91 (t, J = 5.0 Hz, 2H), 3.83 (b, 2H), 3.35 (septet, J = 7.0 Hz, 1H), 2.35 (s, 3H), 1.21 (d, J = 7.0 Hz, 6H). ^{13}C NMR (125 MHz, $CDCl_3$): δ = 156.0, 154.4, 154.2, 144.8, 137.3, 132.9, 129.8, 128.0, 126.8, 126.7, 126.6, 126.1, 125.3, 125.1, 120.9, 114.8, 114.5, 111.5, 105.8, 105.7, 70.3, 70.0, 70.0, 69.4, 69.0, 68.0, 67.9, 67.8, 26.9, 22.7, 21.6. MS (MALDI–TOF) calcd for m/z = 608.244 $[M]^+$, found m/z = 608.371.



Scheme S3. Synthesis of **1**

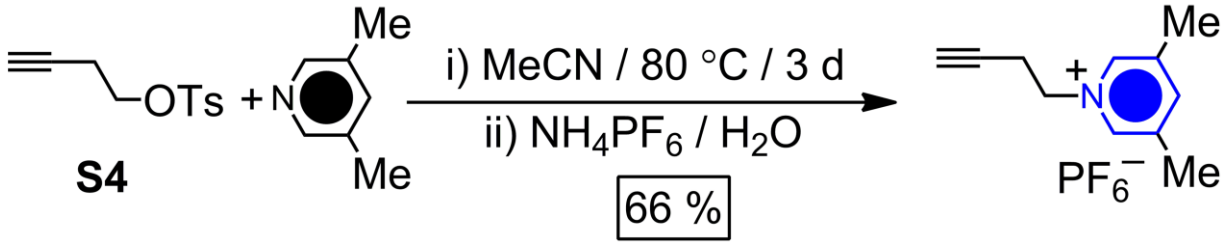
1: **S3** (203 mg, 0.33 mmol) and NaN_3 (130 mg, 2 mmol) were dissolved in dry DMF (50 mL). The reaction mixture was stirred at 80 °C for 16 h. After cooling down to room temperature, the solution was poured into H_2O (200 mL). The resulting mixture was extracted with EtOAc (3 x 20 mL) and the combined organic phases were washed three times with saturated aqueous NaCl solution (3 x 100 mL). After drying ($MgSO_4$), the solvent was removed in vacuo to afford the desired product **1** (157 mg, 98%) as a colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.89 (d, J = 8.5 Hz, 1H), 7.87 (d, J = 8.5 Hz, 1H), 7.35 (t, J = 8.5 Hz, 1H), 7.32 (t, J = 8.5 Hz, 1H), 7.20 (dd, J = 7.5, 1.3 Hz, 1H), 7.13 (td, J = 8.0, 1.5 Hz, 1H), 6.92 (td, J = 8.0, 1.5 Hz, 1H), 6.83–6.80 (m, 3H), 4.28 (t, J = 5.0 Hz, 2H), 4.26 (t, J = 5.0 Hz, 2H), 4.15 (t, J = 5.0 Hz, 2H), 4.04 (t, J = 5.0 Hz, 2H), 3.99 (t, J = 5.0 Hz, 2H), 3.95 (t, J = 5.0 Hz, 2H), 3.77 (t, J = 5.0 Hz, 2H), 3.38 (t, J = 5.0 Hz, 2H), 3.35 (septet, J = 7.0 Hz, 1H), 1.20 (d, J = 7.0 Hz, 6H). ^{13}C NMR (125 MHz, $CDCl_3$): δ = 155.9, 154.2, 154.1, 137.1, 126.7, 126.6, 126.4, 126.0, 125.0, 125.0, 120.7, 114.6, 114.4, 111.4, 105.6, 105.5, 70.2, 70.1, 69.8, 69.7, 67.9, 67.8, 67.6, 50.7, 26.8, 22.6. MS (MALDI–TOF) calcd for m/z = 502.232 $[M + Na]^+$, found m/z = 502.328.



Scheme S4. Synthesis of the [2]pseudorotaxane **D2**·2PF_6⊂**CBPQT**·4PF_6

D2·2PF_6⊂**CBPQT**·4PF_6: A solution of **2** (38 mg, 0.1 mmol), 3,5-dimethyl-1-(but-3-ynyl)-pyridinium hexafluorophosphate (61 mg, 0.2 mmol), **CBPQT**·4PF_6 (110 mg, 0.1 mmol), TBTA (9 mg,0.017 mmol), and $Cu(MeCN)_4PF_6$ (6 mg, 0.017 mmol) in anhydrous Me_2CO (5 mL) was stirred for 24 h at room temperature. The solvent was then evaporated off and the resulting purple solid was purified by column chromatography [SiO_2: 2M NH_4Cl / MeOH / $MeNO_2$ (12 : 7: 1)], then MeOH, Me_2CO and 2% NH_4PF_6 / Me_2CO, respectively. The purple fraction in Me_2CO was collected, and concentrated to a minimum volume, before the crude product was precipitated by the addition of H_2O. The resulting solid was collected by filtration to afford the [2]pseudorotaxane **D2**·2PF_6⊂**CBPQT**·4PF_6 (86 mg, 41%) as a purple powder. ^{1}H NMR (600 MHz, CD_3CN, 233K): δ = 8.90 (d, J = 7.0 Hz, 4H), 8.66 (d, J = 6.0 Hz, 4H), 8.31 (s, 4H), 8.09 (s, 2H), 7.94 (s, 4H), 7.84 (s,

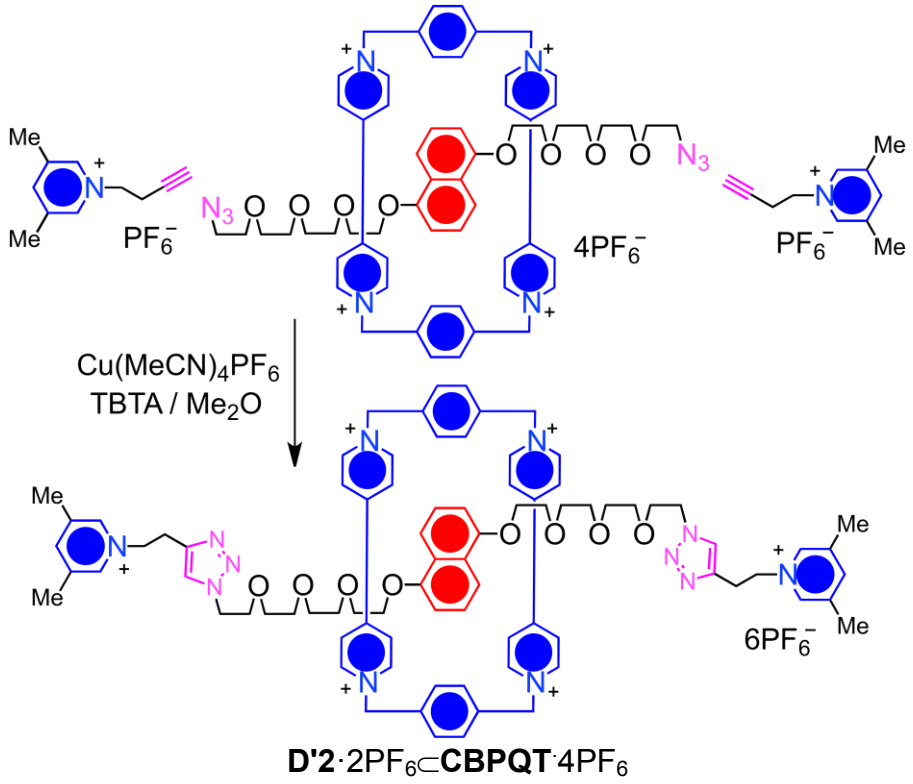
2H), 7.83 (s, 4H), 7.44 (d, J = 7.0 Hz, 4H), 7.12 (d, J = 6.0 Hz, 4H), 6.19 (d, J = 7.8 Hz, 2H), 5.92 (t, J = 7.8 Hz, 2H), 5.90 (d, J = 13.8 Hz, 4H), 5.70 (d, J = 13.8 Hz, 4H), 4.72 (t, J = 4.8 Hz, 4H), 4.65 (t, J = 7.2 Hz, 4H), 4.24–4.18 (m, 12H), 3.31 (t, J = 7.2 Hz, 4H), 2.39 (s, 12 H), 2.28 (d, J = 8.4 Hz, 2H). ^{13}C NMR (125 MHz, CD_3CN): δ = 150.7, 149.0, 146.5, 144.9, 144.8, 143.8, 141.3, 141.1, 138.5, 136.2, 135.7, 131.0, 130.0, 127.7, 126.9, 124.0, 122.9, 107.9, 103.9, 69.7, 68.4, 64.7, 64.3, 60.1, 49.2, 26.3, 17.0. ESI-HRMS calcd for m/z = 1951.4791 $[M - PF_6]^+$, found m/z = 1951.4766.



Scheme S5. Synthesis of 3,5-dimethyl-1-(but-3-ynyl)-pyridinium hexafluorophosphate

3,5-dimethyl-1-(but-3-ynyl)-pyridinium hexafluorophosphate: **S4** (2.24 g, 10 mmol) and 3,5-lutidine (1.07 g, 10 mmol) were dissolved in dry MeCN (50 mL). The reaction mixture was stirred at 80 °C for 3 d. After cooling down to room temperature, the solution was poured into H_2O (200 mL). The resulting aqueous solution was washed three times with CH_2Cl_2 (3 x 100 mL), followed by the addition of NH_4PF_6 (2 g). The white precipitate was collected and washed with Et_2O to give 3,5-dimethyl-1-(but-3-ynyl)-pyridinium hexafluorophosphate (2.01 g, 66%) as a white powder. ^{1}H NMR (500 MHz, CD_3CN): δ = 8.41 (s, 2H), 8.21 (s, 1H), 4.55 (t, J = 6.0 Hz, 2H), 2.91 (td, J = 6.5, 2.5 Hz, 2H), 2.43 (t, J = 2.5 Hz, 1H), 2.19 (s, 6H). ^{13}C NMR (125 MHz, CD_3CN): δ = 146.9, 141.1, 138.5, 77.7, 73.0, 59.0, 20.2, 17.0. ESI-HRMS calcd for m/z = 160.1121 $[M - PF_6]^+$, found m/z = 160.1121.

D'2·2PF_6⊂**CBPQT**·4PF_6: The [2]pseudorotaxane **D'2**·2PF_6⊂**CBPQT**·4PF_6 was prepared using a threading-followed-by-stoppering procedure similar to that used to synthesize its shorter counterpart, namely **D2**·2PF_6⊂**CBPQT**·4PF_6.



Scheme S6. Synthesis of the [2]pseudorotaxane **D'2**·2PF_6⊂**CBPQT**·4PF_6

3. ^{1}H NMR Spectroscopic Characterization

The ^{1}H NMR spectrum of **D2**·2PF_6⊂**CBPQT**·4PF_6 in CD_3CN are presented in Figure S2. The assignments have been made based on ^{1}H–^{1}H gradient-selected double-quantum filtered phase-sensitive COSY (Figure S1), recorded in CD_3CN at 233 K. Some of the key correlation peaks are labeled in the spectrum. The ^{1}H NMR spectrum of the [2]pseudorotaxane **D2**·2PF_6⊂**CBPQT**·4PF_6 recorded in CD_3CN does not undergo remarkable changes for a substantial amount of time (on the order of weeks), an observation indicating that the unthreading reaction of **CBPQT**$^{4+}$ ring is

efficiently prohibited by the Columbic repulsion between the pyridinium-based cationic stopper and the macrocycle.

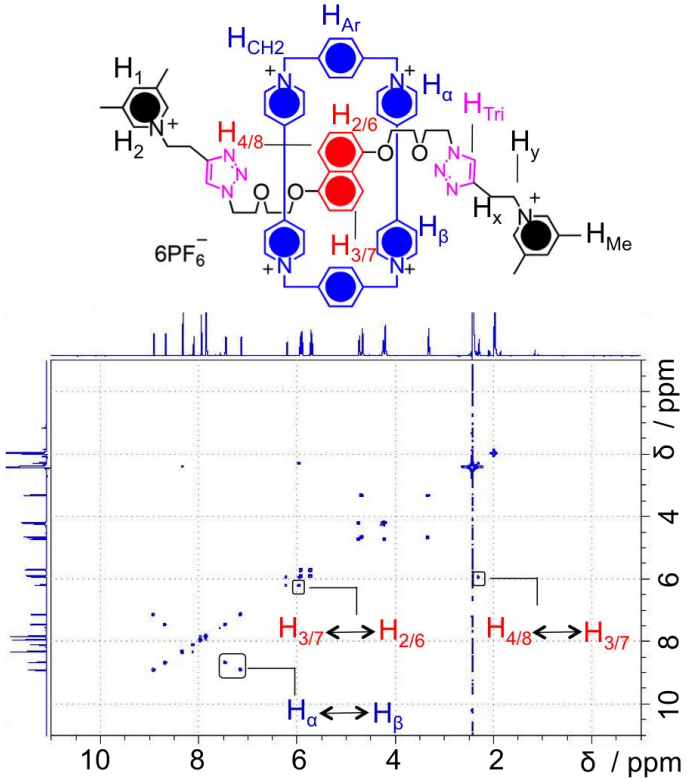


Figure S1. ^{1}H–^{1}H Gradient-selected double-quantum filtered phase-sensitive COSY of **D2**·2PF$_6$⊂**CBPQT**·4PF$_6$ (600 MHz, CD$_3$CN, 233 K).

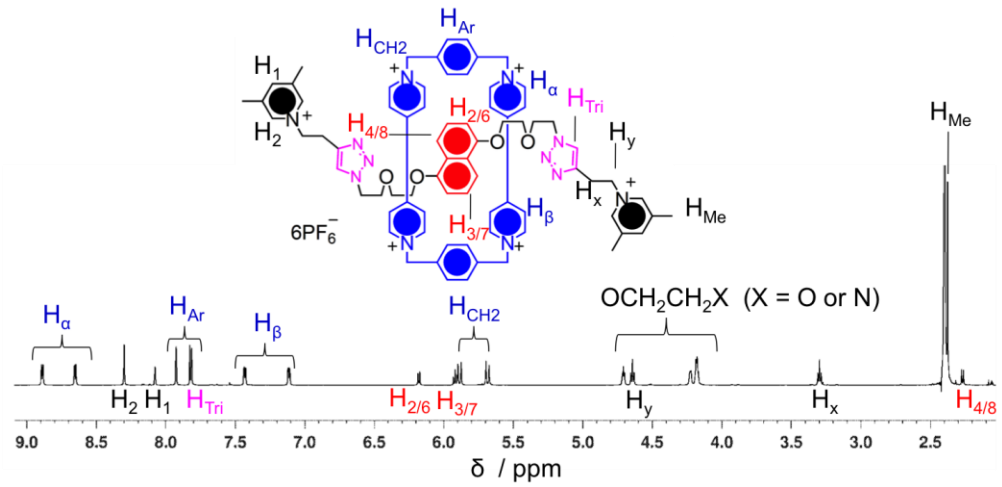


Figure S2. ^{1}H NMR spectrum of **D2**·2PF$_6$⊂**CBPQT**·4PF$_6$ (600 MHz, CD$_3$CN, 233 K).

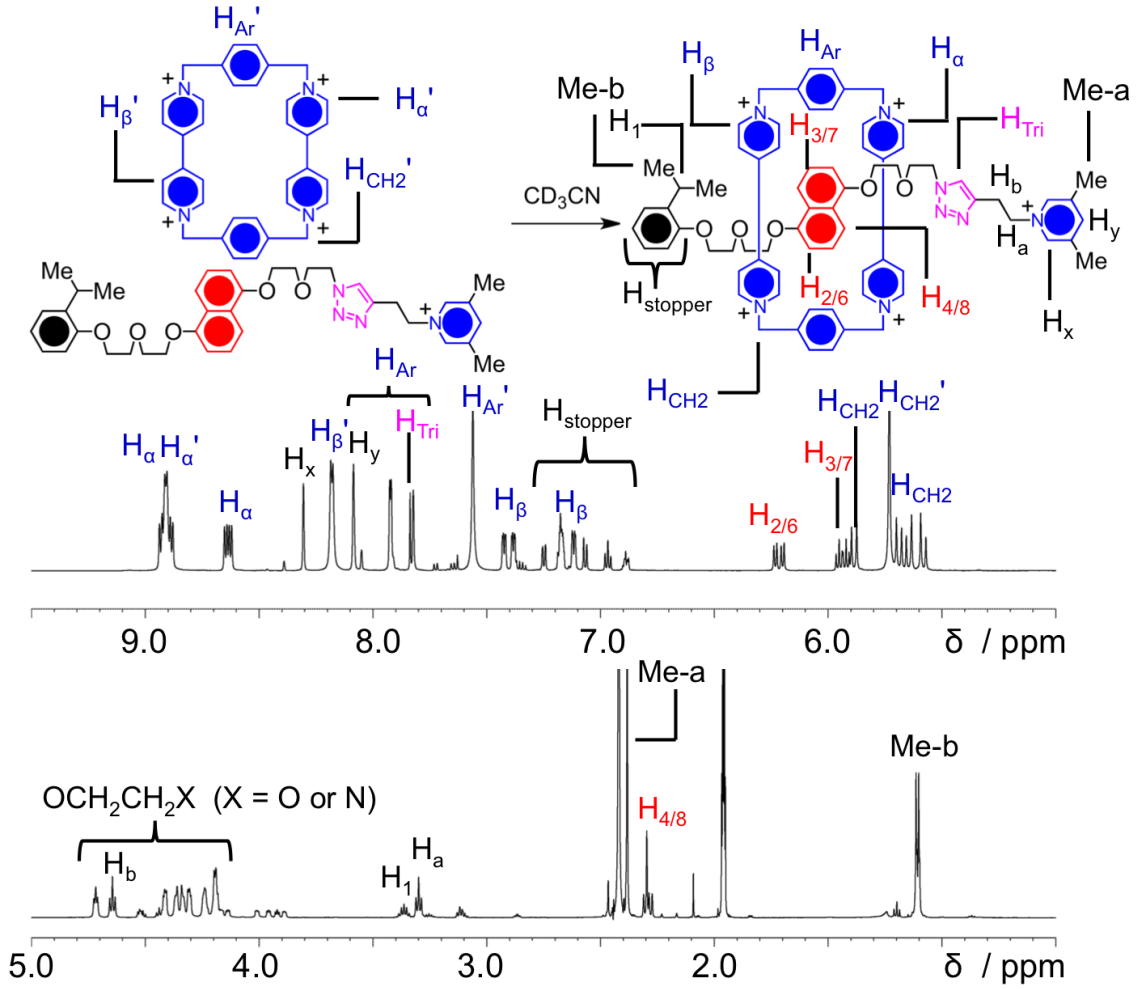


Figure S3. ^{1}H NMR spectrum of **D1**·PF_6⊂**CBPQT**·$4PF_6$ (600 MHz, CD_3CN, 233 K). [**D1**·PF_6]$_0$ = 8.5 × 10^{-3} M; [**CBPQT**·$4PF_6$]$_0$ = 1.2 × 10^{-2} M.

The ^{1}H NMR spectrum of the [2]pseudorotaxane **D1**·PF_6⊂**CBPQT**·$4PF_6$ recorded in CD_3CN at 233 K is presented in Figure S3. The ^{1}H NMR spectra of **D1**·PF_6⊂**CBPQT**·$4PF_6$ in CD_3CN revealed that the $CBPQT^{4+}$ ring encircles the DNP unit of the $\mathbf{D1}^{4+}$ dumbbell.

The ^{1}H NMR spectrum (Figure S6) of the [2]pseudorotaxane $\mathbf{D1}^{+}$⊂$\mathbf{CBPQT}^{4+}$ was recorded after the heterogeneous reduction of the complex with Zn dust, followed by oxidation with atmospheric oxygen. We observed that after the [2]pseudorotaxane $\mathbf{D1}^{+}$⊂$\mathbf{CBPQT}^{4+}$ underwent a reduction/oxidation cycle, its ^{1}H NMR spectrum (Figure S4b) is basically the same as its original

one (Figure S4a), which justifies our assumption that the redox-stimulated association/dissociation of the [2]pseudorotaxane **D1**$^{+}$⊂**CBPQT**$^{4+}$ is almost completely reversible.

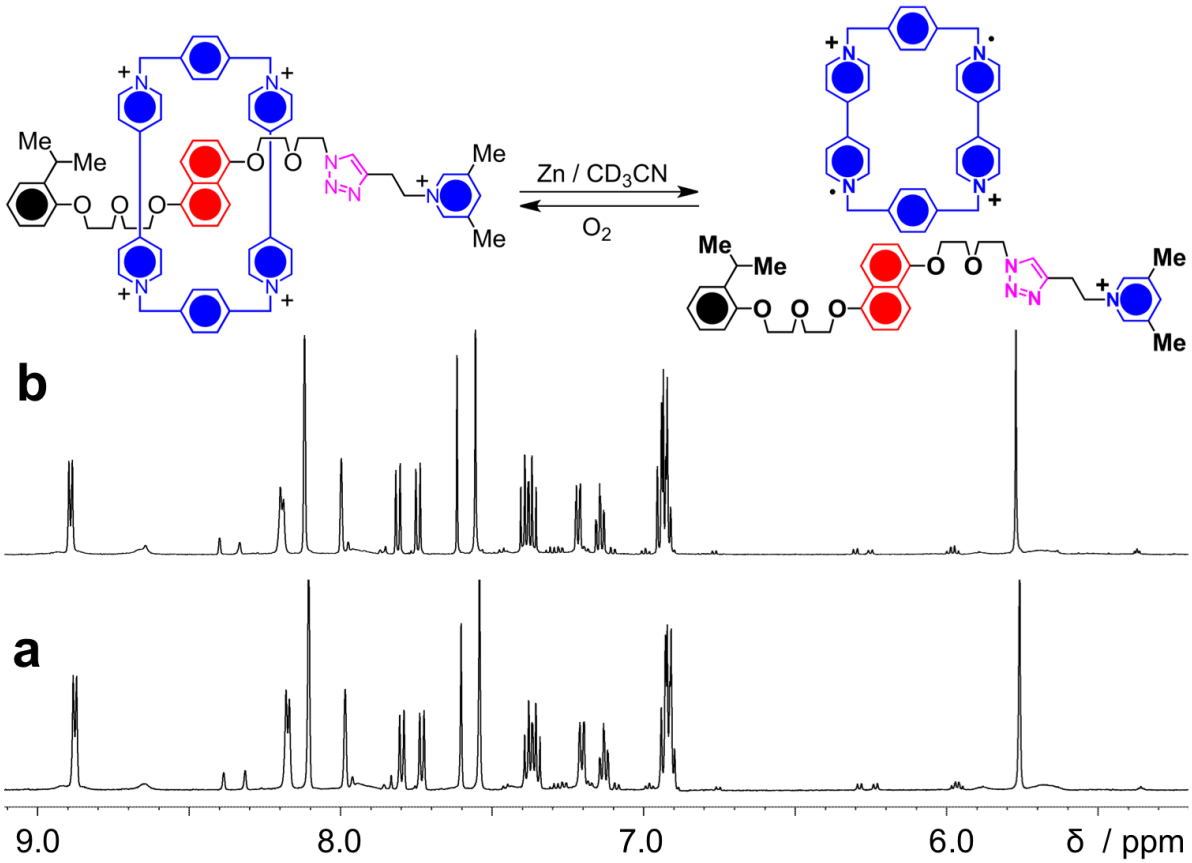


Figure S4. Partial 600 MHz ^{1}H NMR spectra recorded in CD_3CN at 233 K of **a**, the [2]pseudorotaxane **D1**$^{+}$⊂**CBPQT**$^{4+}$ and **b**, the same sample that undergoes heterogenous reduction with Zn dust, followed by exposing the solution to air. [**D1**$^{+}$] = 1.0 × 10^{-2} M, [**CBPQT**$^{4+}$] = 2.0 × 10^{-3} M.

In order to support our hypothesis that light-stimulated reduction of **CBPQT**$^{4+}$ by $Ru(bpy)_3^{3+}$/ptz reducing system can lead to the dissociation of the complex **D'2**$^{2+}$⊂**CBPQT**$^{4+}$, visible light irradiation was carried out to the CD_3CN solution of **D'2**$^{2+}$⊂**CBPQT**$^{4+}$ and its ^{1}H NMR spectrum was recorded. As expected, upon visible light irradiation for 8 h in the presence of both $Ru(bpy)_3^{3+}$ and ptz, free **D'2**$^{2+}$ dumbbell is observed (Figure S5a). This observation indicates that the **CBPQT**$^{4+}$ ring, upon light-stimulated reduction by $Ru(bpy)_3^{3+}$/ptz reducing system, undergoes dethreading over one of the 3,5-dimethylpyridinium terminal units, before the charge-combination

takes place. The dissociation of **D'2**$^{2+}$⊂**CBPQT**$^{4+}$ is not observed when either $Ru(bpy)_3^{3+}$ (Figure S5b) or ptz (Figure S5c) is absent during visible light irradiation, indicating that the $Ru(bpy)_3^{3+}$/ptz reducing system is responsible for the light-stimulated dethreading.

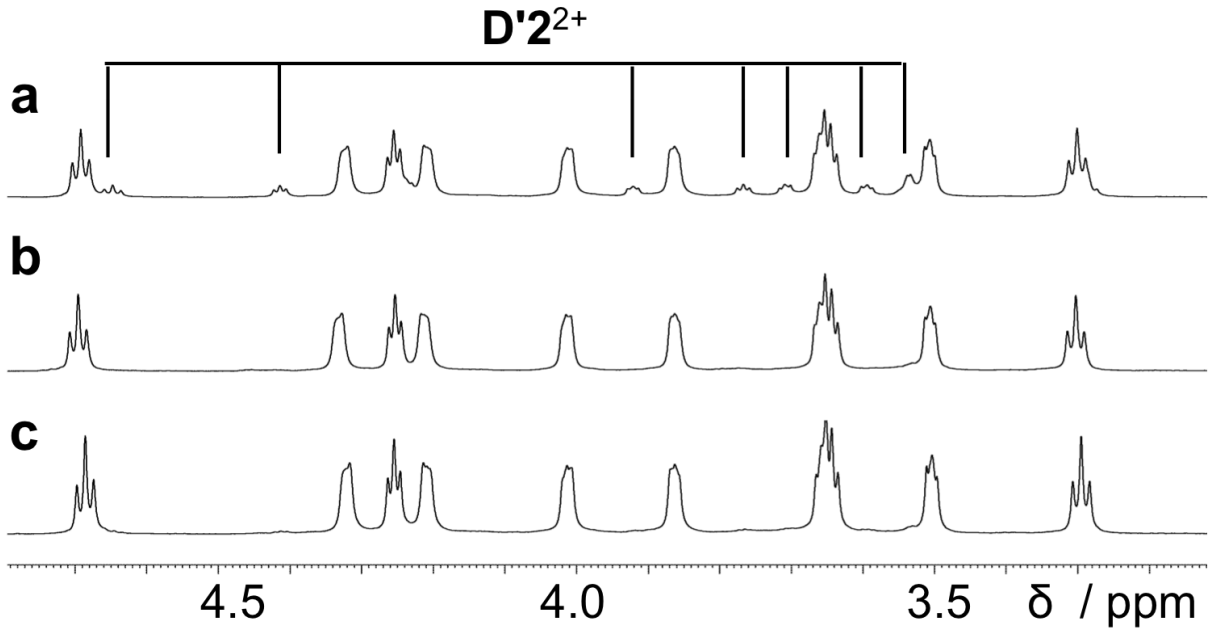


Figure S5. a, Partial 600 MHz ^{1}H NMR spectrum of the [2]pseudorotaxane **D'2**$^{2+}$⊂**CBPQT**$^{4+}$ recorded in CD_3CN at 233 K, after the solution is irradiated with visible light for 8 h when **a**, both $Ru(bpy)_3Cl_2$ and phenothiazine are present; **b**, only $Ru(bpy)_3Cl_2$ is present; and **c**, only phenothiazine is present. Dethreading product, namely, free dumbbell **D'2**$^{2+}$, is observed after visible light irradiation only when both $Ru(bpy)_3Cl_2$ and phenothiazine are present.

4. UV-Vis Absorption Spectra

UV/Vis spectroscopy was employed to evaluate the kinetic parameters controlling the association and dissociation of the **D1**$^+$⊂**CBPQT**$^{4+}$ inclusion complex. The absorption of the charge-transfer band at 520 nm was used as a measure of the concentration of the inclusion complex as a function

of time. A monoexponential increase of the absorbance at 520 nm in the second time range was recorded (Figure S6) for the formation of the $\mathbf{D1}^{+}\subset\mathbf{CBPQT}^{4+}$ inclusion complex. The concentration of $\mathbf{CBPQT}\cdot 4PF_6$ was varied and the corresponding pseudo-first-order rate constants, k_{obs}, were calculated to be 1.10×10^{-2}, 1.39×10^{-2}, 1.68×10^{-2}, 2.10×10^{-2}, 2.47×10^{-2}, 2.88×10^{-2}, 3.27×10^{-2}, and $3.67 \times 10^{-2}\ s^{-1}$, when the corresponding concentrations of $\mathbf{CBPQT}\cdot 4PF_6$ are 4.5×10^{-3}, 6.8×10^{-3}, 9.1×10^{-3}, 11.3×10^{-3}, 13.6×10^{-3}, 15.9×10^{-3}, 18.2×10^{-3}, and 20.5×10^{-2} M, respectively. Based on these data, a plot (Figure 3c in the main text) of k_{obs} versus the concentration of $\mathbf{CBPQT}\cdot 4PF_6$ yields a rate of association $k_f = 1.6 \pm 0.04\ M^{-1}\ s^{-1}$, and a rate of dissociation $k_b = 2.7 \pm 0.5 \times 10^{-3}\ s^{-1}$. The ratio of k_f / k_b ($5.9 \times 10^2\ M^{-1}$) is consistent with the thermodynamic equilibrium constants determined by ^{1}H NMR ($6.0 \times 10^2\ M^{-1}$) spectroscopy. Based on these data, $\Delta G^{\ddagger}_{threading} = 17.2$ kcal mol^{-1} and $\Delta G^{\ddagger}_{dethreading} = 21.0$ kcal mol^{-1} are deduced.

A similar control experiment to measure the kinetic parameters controlling the association and dissociation of **D3** with $\mathbf{CBPQT}^{4+}$ was also conducted (Figure S7) – monitoring the formation of $\mathbf{D3}\subset\mathbf{CBPQT}^{4+}$ by UV/vis spectroscopy. The plot of k_{obs} versus the concentration of $\mathbf{CBPQT}\cdot 4PF_6$ (Figure S9i) yields a rate of association $k_f = 5.71 \pm 0.33\ M^{-1}\ s^{-1}$, and a rate of dissociation $k_b = 8.84 \pm 0.42 \times 10^{-3}\ s^{-1}$. Based on these data, $\Delta G^{\ddagger}_{threading} = 16.9$ kcal mol^{-1} and $\Delta G^{\ddagger}_{dethreading} = 20.6$ kcal mol^{-1} are deduced. The close agreement of the observed kinetics of threading and dethreading for $\mathbf{CBPQT}^{4+}$ with both $\mathbf{D1}^{+}$ and **D3** is consistent with our proposal of directional threading of $\mathbf{CBPQT}^{4+}$ onto $\mathbf{D1}^{+}$ via the 2-isopropylphenyl terminus under oxidative conditions.

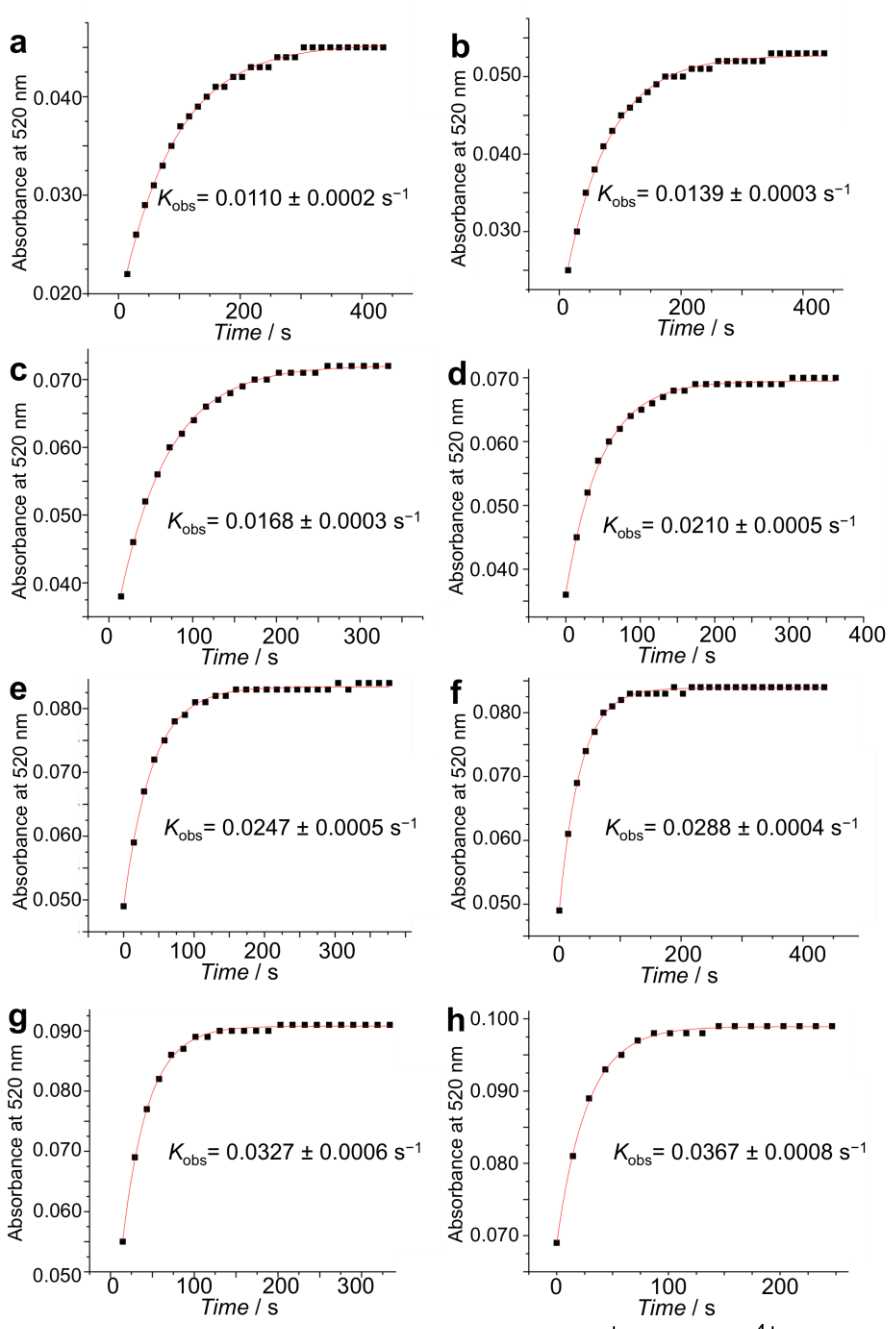


Figure S6. Kinetic trace for the formation of the **D1**$^{+}$⊂**CBPQT**$^{4+}$ inclusion complex obtained by tracking the absorbance at 520 nm in the UV/Vis absorption spectra recorded in MeCN at 298 K when the starting concentration of **CBPQT**$^{4+}$ is **a**, 4.5 × 10^{-3}, **b**, 6.8 × 10^{-3}, **c**, 9.1 × 10^{-3}, **d**, 11.3 × 10^{-3}, **e**, 13.6 × 10^{-3}, **f**, 15.9 × 10^{-3}, **g**, 18.2 × 10^{-3}, and **h**, 20.5 × 10^{-3} M. All the spectra were recorded every 14.5 s in a 2 mm cell-path length cuvette. [**D1**$^{+}$]$_0$ = 1.5 × 10^{-3} M

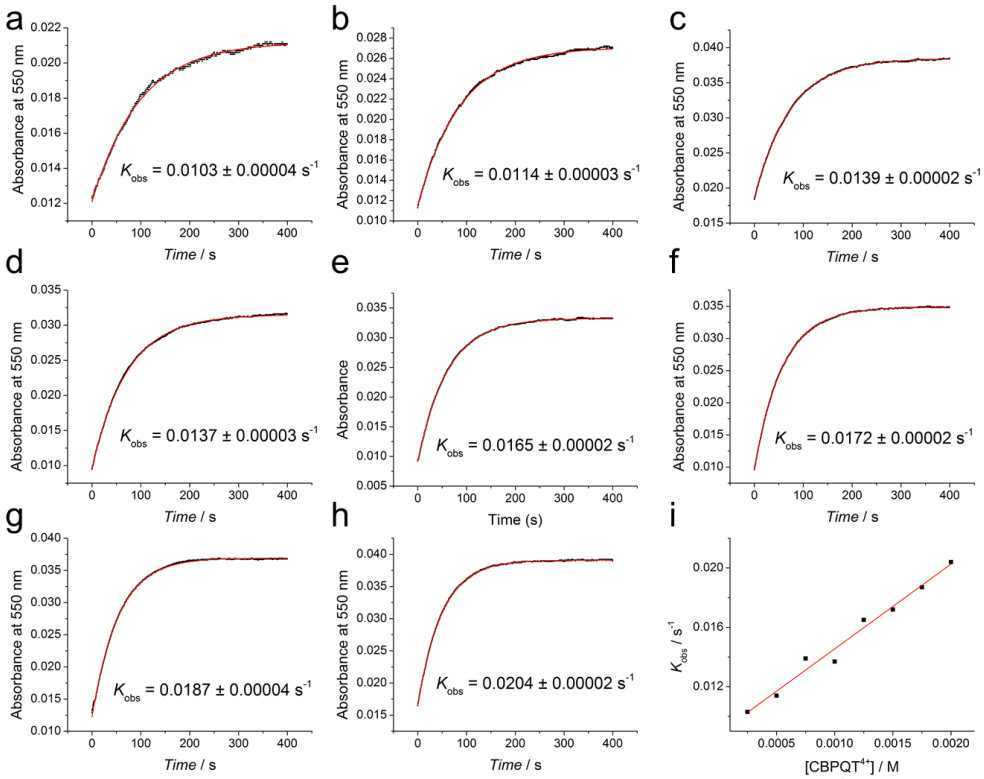


Figure S7. Kinetic traces for the formation of the **D3**⊂**CBPQT**$^{4+}$ inclusion complex obtained by tracking the absorbance at 550 nm in the UV/Vis absorption spectra recorded in MeCN at 298 K when the starting concentration of **CBPQT**$^{4+}$ is **a**, 2.5 × 10^{-4}, **b**, 5.0 × 10^{-4}, **c**, 7.5 × 10^{-4}, **d**, 10.0 × 10^{-4}, **e**, 12.5 × 10^{-4}, **f**, 15.0 × 10^{-4}, **g**, 17.5 × 10^{-4}, and **h**, 20.0 × 10^{-4} M. Spectra were recorded every 0.5 s in a 10 mm cell-path length cuvette. [**D3**]$_0$ = 1.0 × 10^{-4} M. **i**, A plot of the apparent pseudo-first-order rate constant, k_{obs}, versus the concentration of **CBPQT**$^{4+}$.

In order to shed further light on our assumption the [2]pseudorotaxane **D1**$^{+}$⊂**CBPQT**$^{4+}$ undergoes reversible dissociation and association, upon reduction and oxidation, respectively, spectroelectrochemistry (SEC) of a mixture of the dumbbell **D1**$^{+}$, **CBPQT**$^{4+}$ ring and methyl viologen (**V**$^{2+}$) is recorded (Figure S8) upon application of a reductive voltage (–700 mV). Under this reductive condition, the solution of the mixture was observed to have the characteristic maximum absorptions of the BIPY$^{(\bullet+)}$ radical dimers (purple trace, λ_{max} = 560 nm, 1080 nm), indicating the formation of a [2]pseudorotaxane **V**$^{(\bullet+)}$⊂**CBPQT**$^{2(\bullet+)}$, as well as the dissociation of the **D1**$^{+}$⊂**CBPQT**$^{4+}$ complex. Decreasing the potential to 0 mV followed by exposing the solution to air leads to the diminish of the characteristic maximum absorptions of the BIPY$^{(\bullet+)}$ radicals, as

well as the recovery of the DNP⊂**CBPQT**$^{4+}$ charge-transfer band (blue trace, λ_{max} = 520 nm), indicating the reassociation of **D1**$^{+}$⊂**CBPQT**$^{4+}$.

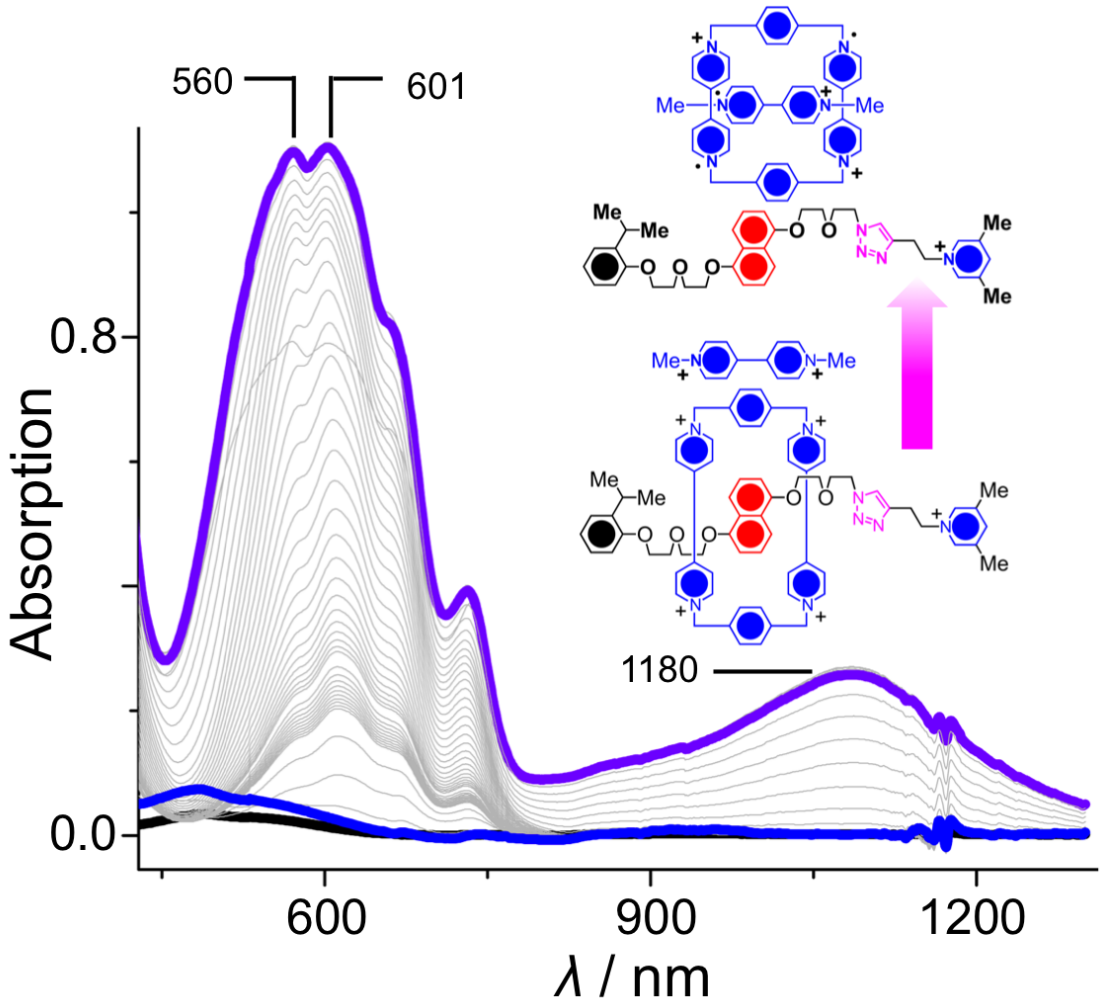


Figure S8. SEC of a 1:2:2 mixture of **CBPQT**$^{4+}$, **D1**$^{+}$ and methyl viologen (**V**$^{2+}$) before (black trace) and after (purple) reduction. Upon reduction, the DNP⊂**CBPQT**$^{4+}$ charge-transfer band disappears while the characteristic maximum absorptions of the (BIPY$^{\bullet+}$)$_2$ radical dimers (λ_{max} = 560 nm, 1080 nm, roughly) is observed. These observations indicate that reduction of the **CBPQT**$^{4+}$ and **V**$^{2+}$ leads to the formation of a **V**$^{\bullet+}$⊂**CBPQT**$^{2(\bullet+)}$ trisradical complex and the dissociation of **D1**$^{+}$⊂**CBPQT**$^{4+}$. Oxidation of the BIPY$^{\bullet+}$ radicals back to their fully oxidized states leads to the recovery of the DNP⊂**CBPQT**$^{4+}$ charge-transfer band (blue trace), whose absorption coefficient is slightly higher than original one, which could be explained by solvent evaporation during the SEC experiment. All data were recorded in MeCN (0.1 M $TBAPF_6$) at room temperature in a quartz cell with a 0.2 cm path length. [**CBPQT**$^{4+}$] = 1.0×10^{-3} M. [**D1**$^{+}$] = 2.0×10^{-3} M. [**V**$^{2+}$] = 2.0×10^{-3} M.

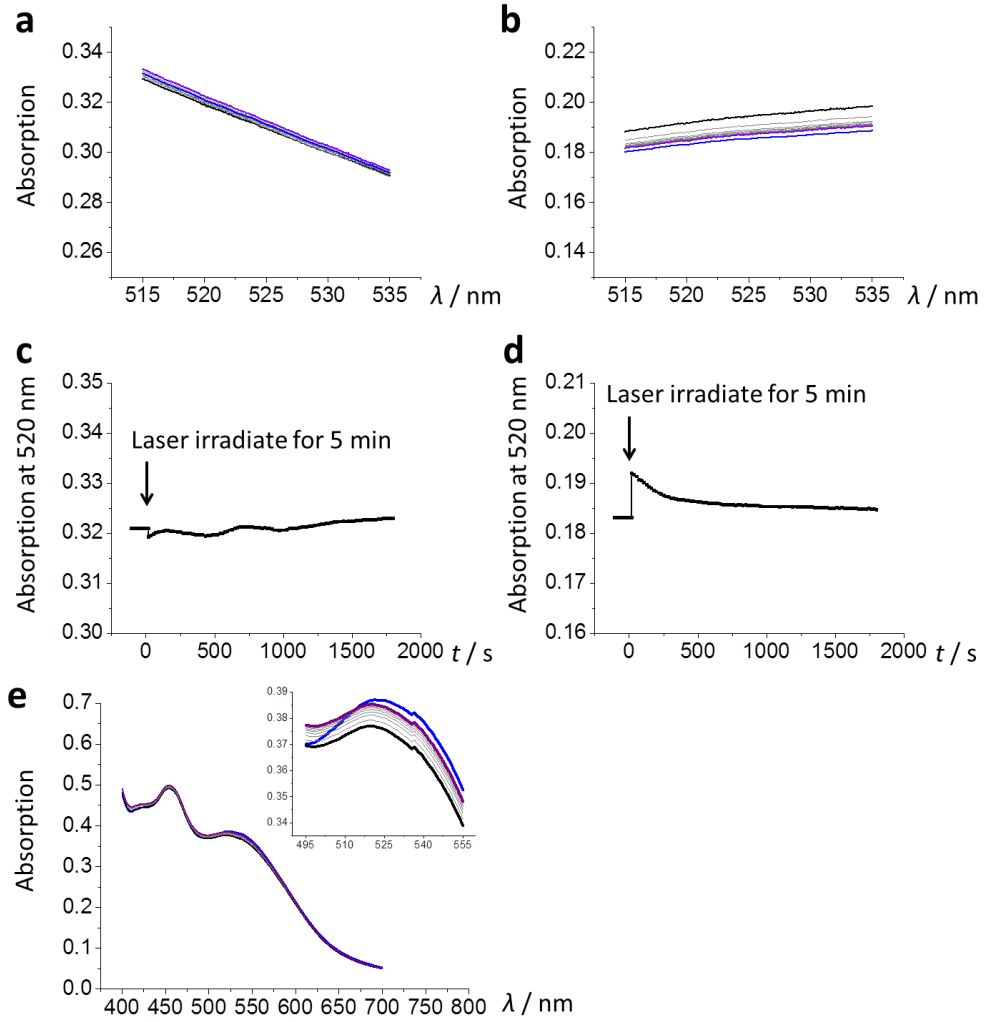


Figure S9. a,**c,** Partial UV/Vis absorption spectra of the MeCN solution of the mixture of **D1**$^{+}$, **CBPQT**$^{4+}$, and $Ru(bpy)_3Cl_2$ recorded (blue trace) after the solution is irradiated with laser at 450 nm for 5 min (black trace), and 30 min after remaining in the dark (purple trace). [**D1**$^{+}$]$_0$ = 1.0 × 10^{-3} M; [CBPQT^{4+}]$_0$ = 2.5 × 10^{-3} M; [$Ru(bpy)_3Cl_2$] = 1.3 × 10^{-4} M. **b**,**d,** Partial UV/Vis absorption spectra of the MeCN solution of the mixture of **D1**$^{+}$, **CBPQT**$^{4+}$, and ptz recorded after the solution is irradiated with laser at 450 nm for 5 min. [**D1**$^{+}$]$_0$ = 1.0 × 10^{-3} M; [CBPQT^{4+}]$_0$ = 2.5 × 10^{-3} M; [ptz] = 8.5 × 10^{-3} M. In each case, the absorbance at 520 nm does not undergo remarkable changes when compared to the change observed when **D1**$^{+}$, **CBPQT**$^{4+}$, $Ru(bpy)_3Cl_2$ and ptz are all present (see Figure 6 in the main text). **e**, Full UV/Vis absorption spectra of of the MeCN solution of the mixture of **D1**$^{+}$, **CBPQT**$^{4+}$, $Ru(bpy)_3Cl_2$ and ptz ([**D1**$^{+}$]$_0$ = 1.0 × 10^{-3} M; [**CBPQT**$^{4+}$]$_0$ = 2.5 × 10^{-3} M; [$Ru(bpy)_3Cl_2$] = 2.6 × 10^{-5} M; [ptz] = 1.7 × 10^{-3} M) recorded before (blue trace) and 40 s after (black trace) the solution has been irradiated with a laser at 450 nm for 5 min and then after being allowed to stand in the dark for 30 min (purple trace).

We have demonstrated in the main text that the [2]pseudorotaxane **D1**$^{+}$⊂**CBPQT**$^{4+}$ underwent dissociation upon laser irradiation at 450 nm in the presence of $Ru(bpy)_3^{2+}$ and ptz (bpy = 2,2'-

bipyridine, ptz = phenothiazine), which act as the photosensitizer and electron relay, respectively. We also observed rethreading of the complex after stopping laser irradiation. In contrast, the dethreading & rethreading were not observed when either $Ru(bpy)_3^{2+}$ (Figure S9a) or ptz (Figure S9b) was absent during laser irradiation, an observation consistent with our NMR results (Figure S5b, S5c). These observations serve as control experiments, which strengthen the assumption that the $Ru(bpy)_3^{2+}$/ptz system is responsible for the light-stimulated dethreading/rethreading.

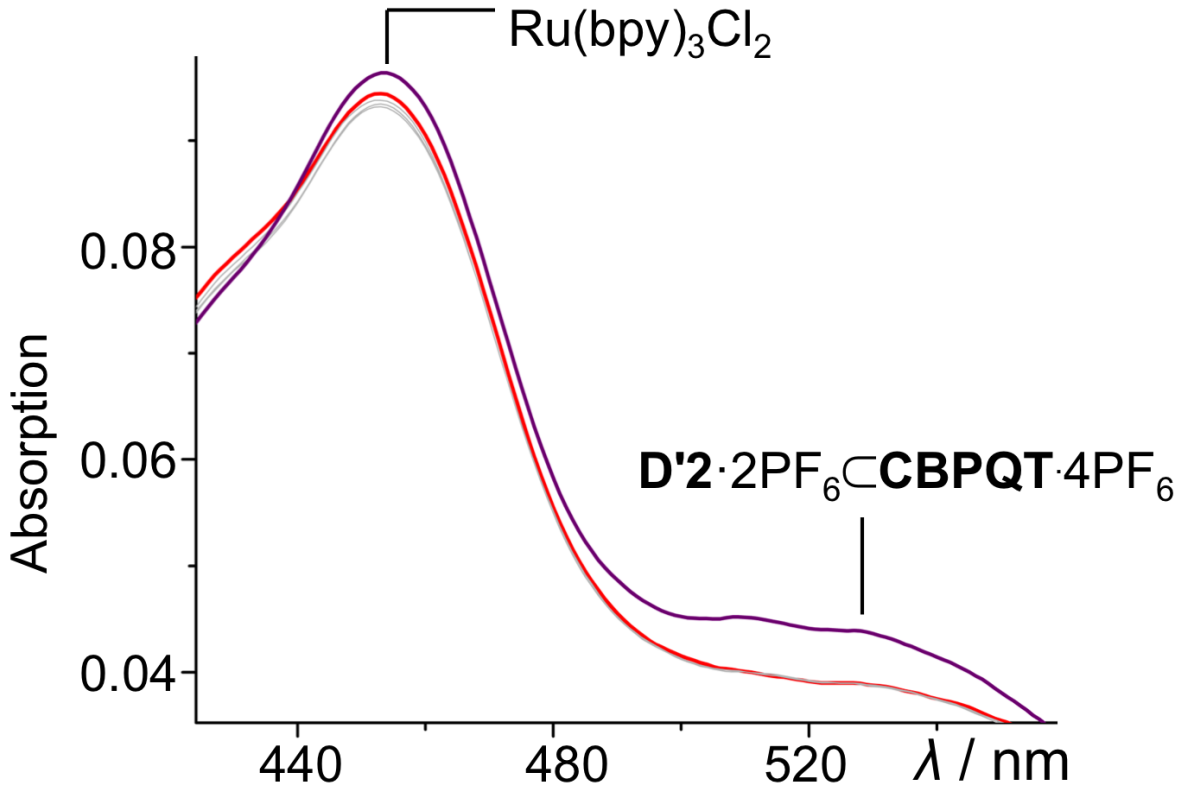


Figure S10. a, UV/Vis absorption spectra of the MeCN solution of the mixture of **D'2**$^{2+}$⊂**CBPQT**$^{4+}$, $Ru(bpy)_3Cl_2$ and phenothiazine recorded before (purple trace) and after (red trace) the solution is irradiated with laser at 450 nm for 5 min. [**D'2**$^{2+}$⊂**CBPQT**$^{4+}$]$_0$ = 5.5 × 10^{-4} M; [$Ru(bpy)_3Cl_2$] = 1.3 × 10^{-4} M; [phenothiazine] = 8.5 × 10^{-3} M.

Light-stimulated dethreading was observed (Figure S10) by employing UV/Vis spectroscopy in the case of the [2]pseudorotaxane **D'2**$^{2+}$⊂**CBPQT**$^{4+}$ in the presence of both $Ru(bpy)_3^{2+}$ and ptz. This observation is consistent with our NMR results (Figure S5a), which further supports our

assumption that the **CBPQT**$^{4+}$ ring, upon light-stimulated reduction by $Ru(bpy)_3^{3+}$/ptz reducing system, undergoes dethreading over one of the 3,5-dimethylpyridinium terminal units, before the charge-combination takes place. After stopping the laser irradiation, rethreading did not occur, an observation which is consistent with the previous results that the 3,5-dimethylpyridinium stoppers in the **D'2**$^{2+}$ dumbbell efficiently prohibit threading of **CBPQT**$^{4+}$, as a result of Coulombic repulsion.

5. Electrochemistry

The observation (Figure S11a) that the two $BIPY^{2+}$ in the [2]pseudorotaxanes BHEEN⊂**CBPQT**$^{4+}$ undergo simultaneous first two-electron reduction can be explained by the fast unthreading process after the first one-electron reduction. Upon reduction of the $BIPY^{2+}$ that is not strongly engaged in π-electron donor-acceptor interactions, the complex BHEEN⊂**CBPQT**$^{(2+)(\bullet+)}$ undergoes fast dissociation, on account of the loss of recognition of the donor-acceptor interactions. As a consequence, the second $BIPY^{2+}$ unit becomes "free" and gets reduced at the same potential as that of the first one. The [2]pseudorotaxane **D4**⊂**CBPQT**$^{4+}$ has a similar redox behavior as that of BHEEN⊂**CBPQT**$^{4+}$ (Figure S11b), because the 3,5-dimethylphenyl terminal groups of the dumbbell **D4** are too small to slow down the association/dissociation of the **D4**⊂**CBPQT**$^{4+}$ complex.

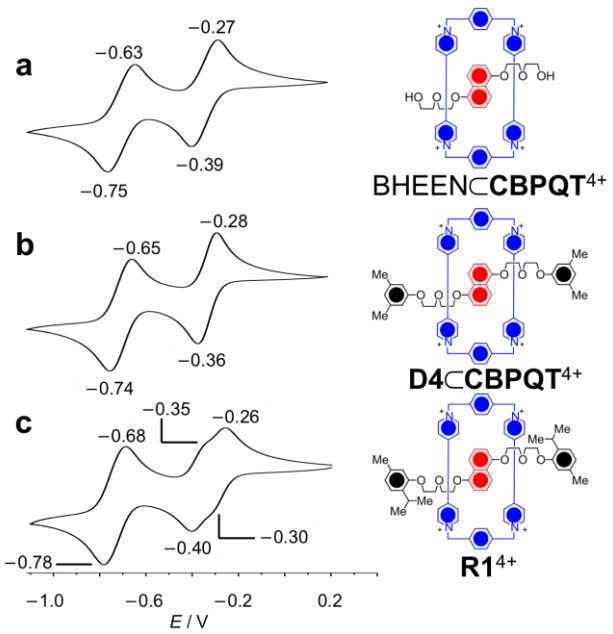


Figure S11. The second scans of the cyclic voltammograms for **a**, BHEEN⊂**CBPQT**$^{4+}$, **b**, **D4**⊂**CBPQT**$^{4+}$, **c**, **R1**$^{4+}$. The voltammograms were recorded under at 298 K, in argon-purged MeCN – concentration: 1 mM and electrolyte: 0.1 M (**TBA**·PF_6). The scan rate was set at 200 mV s^{-1}.

The first two-electron redox process of the **CBPQT**$^{4+}$ component of the [2]rotaxane **R1**$^{4+}$, however, occurs in a stepwise manner (Figure S11c). Upon reduction of the BIPY^{2+} (**CBPQT**$^{4+}$ / **CBPQT**$^{(2+)(\bullet+)}$ (–0.30 V peak potential)) that is not strongly engaged in π-electron donor-acceptor interactions, the mechanical bond of the [2]rotaxane **R1**$^{(2+)(\bullet+)}$ prohibits the dissociation of its two components and thus preserves the π-electron donor-acceptor interactions between the second BIPY^{2+} and the DNP unit, making the reduction of the former occur at a more negative potential (**CBPQT**$^{(2+)(\bullet+)}$ / **CBPQT**$^{2(\bullet+)}$ (–0.40 V peak potential)).

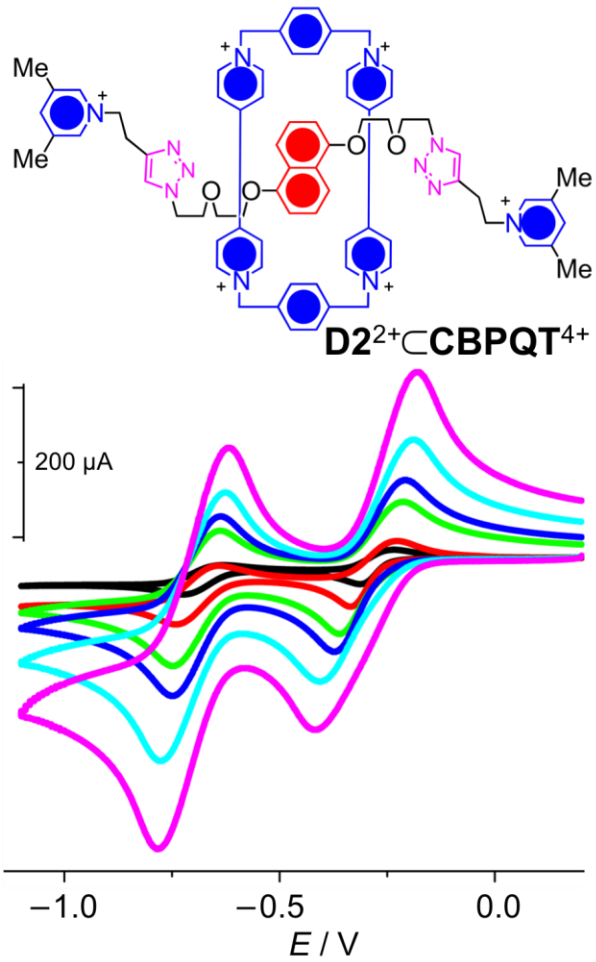


Figure S12. Variable scan rate cyclic voltammetry of the [2]pseudorotaxane **D2**$^{2+}$⊂**CBPQT**$^{4+}$ obtained in MeCN at 298 K with 0.1 M **TBA**·PF_6 as the supporting electrolyte. Black trace: 50 mV s^{-1}; red trace: 200 mV s^{-1}; green trace: 500mV s^{-1}; blue trace: 1000 mV s^{-1}; light-blue trace: 2000 mV s^{-1}; pink trace: 5000 mV s^{-1}.

The [2]pseudorotaxane **D2**$^{2+}$⊂**CBPQT**$^{4+}$, undergoes simultaneous two-electron reductions (Figure S12), indicating that dissociation of this two [2]pseudorotaxane occurs immediately after the reduction of the **CBPQT**$^{4+}$ ring. Even after the scan rate is increased to 5000 mV s^{-1} in the CV experiment, the first two-electron reductions still occur simultaneously. The implication is that, the 3,5-dimethyl pyridinium-based stoppers in the dumbbells **D2**$^{2+}$ and **D1**$^{+}$, cannot slow down the unthreading processes of the reduced states of **CBPQT**$^{4+}$, namely, **CBPQT**$^{2(\bullet+)}$ or **CBPQT**$^{(2+)(\bullet+)}$,

which could be explained by the reduced Columbic repulsion between the stoppers and the macrocycle, resulting from the reduced charge of the latter.

6. DFT Calculations

Computational studies based on density functional theory (DFT) were performed with a view to gaining further insight into the mechanostereoselectivity of the redox-stimulated threading/dethreading of $\mathbf{D1}^{+}\subset\mathbf{CBPQT}^{4+}$. According to the results of these calculations, the $\mathbf{CBPQT}^{4+}$ ring has to overcome energy barriers ($\Delta E^{\ddagger}$) of 34.3 and 17.2 kcal mol^{-1} (Figure 6a) in order to thread onto dumbbell $\mathbf{D1}^{+}$ from the 3,5-dimethylpyridinium and 2-isopropylphenyl ends, respectively. The theoretical $\Delta E^{\ddagger}$ value for the 2-isopropylphenyl barrier matches up exactly with the experimental data, whereas that of the 3,5-dimethylpyridinium end is considerably higher (34.3 *vs* 24.3 kcal mol^{-1}) than we determined (Figure 6b) using ^{1}H NMR spectroscopy. This discrepancy is most likely an upshot of interactions between ions in solution which were not accounted for by the computational model. In a CD_3CN solution of $\mathbf{D1}^{+}\subset\mathbf{CBPQT}^{4+}$, both $\mathbf{D1}^{+}$ and $\mathbf{CBPQT}^{4+}$ are surrounded by PF_6^{-} counterions which serve to neutralize the positive charges partially, thereby sating the Coulombic repulsion between the two cationic species to some extent.

In the case of the dicationic $\mathbf{CBPQT}^{2(\bullet+)}$ ring, the values of $\Delta E^{\ddagger}$ for its dissociation from the 3,5-dimethylpyridinium and 2-isopropylphenyl ends of the $\mathbf{D1}^{+}$ dumbbell are 23.5 and 26.6 kcal mol^{-1}, respectively, which translate (Figure 6c) to peaks 18.2 and 21.3 kcal mol^{-1} above the energy of the non-complexed components. The result of this calculation are consistent with dissociation of $\mathbf{D1}^{+}\subset\mathbf{CBPQT}^{2(\bullet+)}$ occuring preferentially at the 3,5-dimethylpyridinium end.

In the case of the **CBPQT**$^{(2+)(\bullet+)}$ ring, the values of $\Delta E^{\ddagger}$ for it to dethread from the 3,5-dimethylpyridinium and 2-isopropylphenyl ends are 38.1 and 28.5 kcal mol^{-1}, respectively, i.e., 31.6 and 22.0 kcal mol^{-1} in threading terms (Figure 6b). The energy barrier (31.6 kcal mol^{-1}) for the **CBPQT**$^{(2+)(\bullet+)}$ ring to slip over the 3,5-dimethylpyridinium end is smaller than that (34.3 kcal mol^{-1}) for the **CBPQT**$^{4+}$ ring — a situation which is not surprising since the Coulombic repulsion between the reduced ring and the 3,5-dimethylpyridinium end is a lot less. According to DFT calculations, the energy barrier for **CBPQT**$^{(2+)(\bullet+)}$ ring to slip over the 3,5-dimethylpyridinium end is larger by 9.6 kcal mol^{-1} than that presented by the 2-isopropylphenyl end, an observation which is inconsistent with the CV experiments. This inconsistency can be explained by the fact that the effect of counterions is not considered in the calculations, which overestimate the Coulombic repulsion between the ring and the charged ends of the dumbbell.

This material includes atomic coordinates and energies of TS and ground state in three different oxidation states given in this study. At infinite separation, the **CBPQT**$^{(n+)}$ rings dissociated from the dumbbell units favors encapsulation of two CH_3CN molecules. These geometries and corresponding energies are also provided. The scans of potential energy surfaces are carried out by constraining the z coordinate of the N atom on the pyridinium ring or the center C atom of the isopropyl group (marked in the atomic coordinates) relative to the center of **CBPQT**$^{(n+)}$, the origin, defined by four C atoms in methylene linkers. The geometries were optimized in Poisson-Boltzmann solvation model[S6] for acetonitrile (ε=37.5 and R_0= 2.18 Å) at the level of M06-HF/6-31G* with Jaguar 7.5[S7]. The scans for the **CBPQT**$^{(n+)}$ moving on **D1**$^{+}$ were carried out by fixing the relative shift between the center of **CBPQT**$^{(n+)}$, which was defined as the geometric average of its four methylene carbons, and the secondary carbon of isopropyl group and the nitrogen atom of pyridinium, respectively. The binding energies of **D1**$^{+}\subset$**CBPQT**$^{(n+)}$ complexes were corrected by

deducting the cost to remove two CH_3CN solvent molecules from the cavity of **CBPQT**$^{(n+)}$, which are 9.9, 8.9 and 6.0 Ha for n=2,3 and 4. Energy has unit in Hartree.

D1^{+}
-2070.69513501178
H 0.18394 -3.05662 -1.68276
C 0.06407 -1.97809 0.14649
C 0.05033 -0.68875 0.75432
C 0.17467 -2.08246 -1.21155
C -0.07900 -0.53397 2.17512
H -0.01672 -2.85586 0.77072
C 0.15638 0.47133 -0.03903
C 0.27919 -0.92742 -2.03564
C -0.10267 0.71261 2.74680
H 0.36386 -1.04864 -3.10616
H -0.20464 0.83642 3.81534
C 0.13341 1.76181 0.56651
C 0.27427 0.31739 -1.46052
C 0.00581 1.86715 1.92277
O 0.37007 1.48464 -2.14971
C 0.32226 1.42625 -3.56480
H 1.18076 0.88010 -3.95884
H -0.60043 0.94267 -3.89133
O -0.17530 -1.69945 2.86662
C -0.30394 -1.62118 4.27609
H 0.55832 -1.11077 4.70874
H -1.21756 -1.08827 4.54593
H -0.01631 2.84156 2.39303
H 0.21334 2.63893 -0.05881
C 0.34097 2.86591 -4.07281
H 1.31743 3.32277 -3.89687
H -0.42953 3.45214 -3.56674
O 0.06754 2.76832 -5.45760
C 0.19678 3.97265 -6.18094
H -0.34485 4.78620 -5.69242
H 1.24690 4.25384 -6.29228
C -0.41394 3.65285 -7.54991
H 0.04736 2.74819 -7.93746
H -1.49008 3.51728 -7.47661
N -0.13213 4.69462 -8.53298
C -0.65003 5.93494 -8.65258
C -0.04460 6.44435 -9.78178
N 0.79151 5.49055 -10.25364

N	0.72885	4.44924	-9.49345
H	-1.37815	6.33205	-7.96520
C	-0.22509	7.75449	-10.50530
H	-1.09954	7.69670	-11.15659
H	-0.38068	8.56044	-9.78847
C	1.02326	8.03569	-11.36215
H	1.89791	8.23476	-10.74808
H	1.23586	7.20402	-12.02612
C	0.24670	11.42260	-13.73188
C	0.75155	11.59154	-12.43727
C	1.01289	10.45274	-11.69824
N	0.78715	9.23005	-12.21350
C	0.30614	9.06349	-13.45245
C	0.01888	10.15567	-14.26236
H	0.03003	12.29868	-14.33334
H	1.40644	10.48303	-10.69125
H	0.15856	8.04353	-13.78136
C	-0.36940	-3.04910	4.81309
H	-1.23091	-3.57418	4.39398
H	0.54339	-3.59179	4.55655
O	-0.49569	-2.89823	6.21284
C	-0.55427	-4.09875	6.95800
H	-1.42357	-4.69656	6.67347
H	0.35225	-4.69226	6.81840
C	-0.67372	-3.64414	8.41053
H	0.19350	-3.03205	8.66557
H	-1.58322	-3.05179	8.52699
O	-0.72264	-4.80186	9.22432
C	-1.00061	-4.42785	13.34694
C	-0.92474	-5.68085	12.72908
C	-0.83019	-5.80912	11.34726
C	-0.81437	-4.62929	10.57492
C	-0.88553	-3.37424	11.17659
C	-0.97949	-3.27994	12.56803
H	-1.07195	-4.35971	14.42444
H	-0.93492	-6.57007	13.34575
H	-0.86803	-2.47168	10.58243
H	-1.03380	-2.30207	13.02899
C	-0.78062	-7.15767	10.64030
H	-0.08336	-7.05882	9.80786
C	-0.29363	-8.29990	11.54661
H	0.65867	-8.05018	12.01765
H	-1.02474	-8.51998	12.32750
H	-0.16164	-9.20146	10.94617
C	-2.17132	-7.49283	10.05834
H	-2.89763	-7.57719	10.86971

H -2.49532 -6.71141 9.37128
H -2.13316 -8.44258 9.52109
C 0.99929 12.97049 -11.86000
H 1.42142 12.89686 -10.85957
H 1.69089 13.51623 -12.50210
H 0.05835 13.51938 -11.81166
C -0.50547 9.93574 -15.66786
H -0.89804 10.86818 -16.06866
H 0.30199 9.58507 -16.31223
H -1.29680 9.18659 -15.66081

$2CH_3CN\subset$**CBPQT**$^{2(\bullet+)}$
-1874.84758061231
H -4.92853 -1.66945 -2.95507
H 5.51751 1.65810 -3.00529
H 2.18996 -1.47372 -3.06719
H -1.60602 1.44671 -3.33030
H -4.12778 -3.24132 -2.78009
H 4.72663 3.23953 -3.14137
H 4.29998 -0.27611 -2.95233
H -3.71825 0.27293 -3.08322
C 2.16294 -0.39584 -3.00993
C -1.58031 0.39076 -3.10668
C -2.77739 -0.24940 -2.98242
C 3.35879 0.25540 -2.95574
C -0.34222 -0.32007 -2.97053
C 0.92415 0.32727 -3.01388
H 0.38092 -2.37764 -2.67890
H 0.20141 2.40488 -3.07825
C -0.47893 -1.73231 -2.77225
C 1.06103 1.75322 -3.04419
N -2.85576 -1.58742 -2.74682
N 3.43562 1.61406 -2.92267
C -1.70610 -2.31062 -2.65244
C 2.28614 2.34275 -2.97999
H -1.82225 -3.37023 -2.47524
H 2.40296 3.41725 -2.96450
C -4.15391 -2.21483 -2.41983
C 4.71595 2.28479 -2.61940
C -4.36622 -2.15915 -0.91336
C 4.83096 2.47557 -1.11304
H -5.29947 -0.21719 -0.94225
H 5.53274 0.46938 -0.75040
H -3.52822 -4.10863 -0.54937
H 4.19707 4.53124 -1.13726
C -4.91121 -1.01722 -0.32262

C 5.21350 1.40316 -0.30229
C -3.92002 -3.20190 -0.10320
C 4.46790 3.68233 -0.52028
C -4.94721 -0.89404 1.06344
C 5.18086 1.52343 1.08207
C -3.95444 -3.07801 1.28452
C 4.43571 3.80330 0.87009
H -5.36560 -0.00009 1.51152
H 5.47490 0.68226 1.69889
H -3.58896 -3.88970 1.90267
H 4.14004 4.74449 1.31895
C -4.43653 -1.91024 1.87402
C 4.76566 2.71798 1.67734
C -4.30019 -1.69470 3.37500
C 4.57905 2.78787 3.18739
H -1.98121 -2.80999 3.75162
H 2.26153 3.96819 3.24216
N -3.01774 -1.01103 3.64866
N 3.27960 2.18083 3.54014
C -1.86840 -1.73528 3.73921
C 2.13544 2.91117 3.42946
H 4.12617 0.32247 3.92876
H -3.88557 0.87610 3.60276
H -5.09961 -1.06809 3.76508
H 5.35521 2.23446 3.71233
C -2.94305 0.34818 3.64135
C 3.19041 0.84842 3.80192
H -4.29401 -2.64001 3.91390
H 4.57449 3.81726 3.54011
C -0.64595 -1.14006 3.81002
C 0.90350 2.34298 3.54508
H 0.21333 -1.78924 3.87645
H 0.04907 2.99524 3.44745
C 1.98825 0.21767 3.91658
C -1.74990 1.00609 3.69837
C -0.51124 0.28552 3.75680
C 0.75636 0.93174 3.74561
H 2.00446 -0.83436 4.15637
H -1.78165 2.08460 3.71665
C 1.73924 0.29085 0.41777
N 1.59958 1.42390 0.30762
C 1.90648 -1.16870 0.56195
H 2.47286 -1.37097 1.46847
H 0.91397 -1.61339 0.62200
H 2.44356 -1.54912 -0.30402
N -1.46092 -0.82675 0.43556

C -1.69247 0.29536 0.39293
C -1.97852 1.74245 0.34430
H -1.16804 2.26877 0.84420
H -2.03730 2.05462 -0.69541
H -2.92451 1.93725 0.84609

2CH_3CN⊂**CBPQT**$^{(2+)(\bullet+)}$
-1874.70137435663
H -4.91845 -1.68045 -2.95750
H 5.46634 1.65865 -3.00889
H 2.15274 -1.44507 -3.32797
H -1.59736 1.36884 -3.61877
H -4.11056 -3.25204 -2.77631
H 4.67240 3.24320 -3.13667
H 4.28489 -0.23202 -3.11425
H -3.73632 0.19536 -3.28382
C 2.12949 -0.37750 -3.16592
C -1.58016 0.34059 -3.28606
C -2.79205 -0.30317 -3.11581
C 3.33794 0.28569 -3.05893
C -0.38913 -0.35054 -3.03523
C 0.93447 0.34526 -3.07008
H 0.39630 -2.30523 -2.47276
H 0.14076 2.36489 -2.85239
C -0.47324 -1.69857 -2.67944
C 1.01308 1.73312 -2.93292
N -2.83877 -1.58981 -2.73351
N 3.37800 1.61642 -2.87867
C -1.71285 -2.29111 -2.53587
C 2.25053 2.34102 -2.83569
H -1.82191 -3.32504 -2.24153
H 2.35474 3.40774 -2.69535
C -4.15511 -2.22880 -2.41174
C 4.68449 2.29565 -2.60402
C -4.35437 -2.16126 -0.90606
C 4.80844 2.48236 -1.10015
H -5.25116 -0.20072 -0.93974
H 5.51696 0.47569 -0.74607
H -3.56096 -4.13096 -0.54066
H 4.17661 4.54087 -1.12471
C -4.87845 -1.00748 -0.31940
C 5.19912 1.40865 -0.29533
C -3.92903 -3.21333 -0.09689
C 4.44873 3.69111 -0.50960
C -4.91612 -0.88483 1.06661
C 5.17405 1.53022 1.08885

C	-3.96338	-3.08700	1.29093
C	4.42182	3.81034	0.88067
H	-5.32166	0.01530	1.51327
H	5.47312	0.69024	1.70457
H	-3.61735	-3.90648	1.90950
H	4.12586	4.75089	1.32985
C	-4.42595	-1.91087	1.87884
C	4.75644	2.72400	1.68479
C	-4.29881	-1.70433	3.38237
C	4.57066	2.79438	3.19556
H	-1.97840	-2.82518	3.74894
H	2.24589	3.95936	3.20944
N	-3.01719	-1.02596	3.66472
N	3.27270	2.18312	3.54777
C	-1.86610	-1.75028	3.74209
C	2.12521	2.90478	3.41324
H	4.12678	0.33743	3.97922
H	-3.88636	0.86254	3.64896
H	-5.09985	-1.07852	3.77076
H	5.34922	2.24470	3.72035
C	-2.94381	0.33350	3.67105
C	3.18914	0.85473	3.83223
H	-4.29890	-2.65378	3.91395
H	4.56300	3.82459	3.54556
C	-0.64318	-1.15562	3.81195
C	0.89574	2.33120	3.52958
H	0.21702	-1.80478	3.87251
H	0.03897	2.97750	3.41491
C	1.98940	0.21839	3.94816
C	-1.75050	0.98930	3.72632
C	-0.50960	0.27081	3.76717
C	0.75506	0.92234	3.75271
H	2.00835	-0.82834	4.21330
H	-1.78183	2.06775	3.76301
C	1.79182	0.20365	0.42297
N	1.69391	1.32280	0.18783
C	1.89788	-1.24202	0.70652
H	2.42713	-1.37999	1.64669
H	0.88675	-1.64007	0.77384
H	2.44675	-1.72507	-0.09930
N	-1.44395	-0.71067	0.28323
C	-1.64024	0.41854	0.33992
C	-1.88979	1.87214	0.40108
H	-1.05229	2.34593	0.91160
H	-1.96933	2.26238	-0.61240
H	-2.81854	2.05175	0.94071

$2CH_3CN\subset$**CBPQT**$^{4+}$
-1874.54703752211
H -4.82469 -1.96099 -2.99168
H 5.39431 1.80503 -3.08363
H 2.19342 -1.38279 -3.72181
H -1.59901 1.10477 -3.99674
H -3.96102 -3.47959 -2.66769
H 4.52992 3.35774 -3.08793
H 4.29005 -0.08860 -3.46555
H -3.70691 -0.14130 -3.61191
C 2.14243 -0.34407 -3.42590
C -1.56257 0.13022 -3.52998
C -2.74860 -0.55344 -3.32914
C 3.32404 0.36649 -3.29647
C -0.35984 -0.45927 -3.13291
C 0.92737 0.29716 -3.17065
H 0.50803 -2.27121 -2.29964
H 0.03690 2.21748 -2.67387
C -0.38728 -1.75425 -2.61336
C 0.94163 1.66039 -2.86746
N -2.75001 -1.77325 -2.76776
N 3.30910 1.66103 -2.94032
C -1.60311 -2.38548 -2.43622
C 2.15211 2.31669 -2.75849
H -1.67792 -3.37497 -2.00898
H 2.21871 3.36320 -2.50191
C -4.04484 -2.42981 -2.39765
C 4.58962 2.37488 -2.62715
C -4.26100 -2.23863 -0.90312
C 4.72969 2.45828 -1.11262
H -5.25623 -0.33721 -1.10807
H 5.64983 0.51721 -0.91896
H -3.38361 -4.13331 -0.36503
H 3.91413 4.44808 -0.96904
C -4.85633 -1.07257 -0.41958
C 5.25210 1.37924 -0.39628
C -3.79949 -3.20022 -0.00377
C 4.27869 3.58486 -0.42507
C -4.94273 -0.84906 0.95352
C 5.27605 1.40920 0.99695
C -3.86976 -2.96880 1.36784
C 4.28933 3.60827 0.96895
H -5.42716 0.04873 1.31895
H 5.70497 0.57497 1.53954
H -3.49830 -3.72036 2.05382

H 3.92215 4.48499 1.48854
C -4.41835 -1.78149 1.85136
C 4.76365 2.51125 1.68618
C -4.39047 -1.48516 3.34518
C 4.66802 2.49175 3.20686
H -2.27693 -2.63605 4.35994
H 2.50689 3.79600 3.88085
N -3.07362 -0.85086 3.67729
N 3.33724 1.92016 3.59411
C -2.06066 -1.60196 4.13206
C 2.30279 2.73502 3.84515
H 4.06372 -0.01275 3.43604
H -3.77562 1.00978 3.10927
H -5.16760 -0.78451 3.64011
H 5.43050 1.86130 3.65724
C -2.90074 0.45604 3.41934
C 3.17618 0.58639 3.58629
H -4.46831 -2.39030 3.94121
H 4.72361 3.49076 3.63034
C -0.79410 -1.06380 4.29222
C 1.02871 2.22683 4.04170
H -0.01488 -1.70737 4.67528
H 0.23321 2.92462 4.26126
C 1.92606 0.02267 3.75146
C -1.65810 1.04420 3.54397
C -0.56556 0.27053 3.95247
C 0.81470 0.85144 3.94334
H 1.84157 -1.05320 3.69304
H -1.56346 2.09191 3.29523
C 2.04882 0.46968 0.52689
N 1.67027 1.55145 0.57261
C 2.50845 -0.93404 0.48780
H 3.32762 -1.06064 1.19232
H 1.67418 -1.57816 0.75858
H 2.85913 -1.17015 -0.51419
N -1.46640 -0.19133 0.15448
C -1.97705 0.83558 0.16174
C -2.63259 2.15950 0.19937
H -1.94327 2.88304 0.63045
H -2.89667 2.45700 -0.81283
H -3.53446 2.09662 0.80585

D1^{+}⊂**CBPQT**$^{2(\bullet+)}$ at DNP
-3680.11500274035
H 0.01766 -2.83891 -1.31231
C -0.03947 -1.76281 0.51293

C	-0.05457	-0.47328	1.11559
C	0.00864	-1.86609	-0.84402
C	-0.13115	-0.33750	2.53616
H	-0.06852	-2.63724	1.14261
C	-0.00621	0.69023	0.32359
C	0.04498	-0.71070	-1.67192
C	-0.14239	0.90334	3.12203
H	0.07800	-0.83944	-2.74390
H	-0.19869	1.01703	4.19552
C	-0.01864	1.97190	0.93653
C	0.04548	0.53483	-1.10386
C	-0.08091	2.05984	2.30114
O	0.08687	1.69150	-1.82105
C	0.06720	1.55218	-3.22494
H	0.92725	0.97512	-3.57127
H	-0.85000	1.05354	-3.54775
O	-0.19458	-1.51418	3.21456
C	-0.33218	-1.46093	4.61908
H	0.53501	-0.97938	5.07534
H	-1.23694	-0.91594	4.89713
H	-0.08988	3.02767	2.78331
H	0.02152	2.85528	0.31146
C	0.11419	2.94265	-3.84574
H	1.09307	3.39946	-3.67902
H	-0.66294	3.57472	-3.41073
O	-0.11962	2.74203	-5.22572
C	0.13230	3.86949	-6.03427
H	-0.37750	4.75477	-5.64531
H	1.20467	4.07116	-6.09938
C	-0.41187	3.50476	-7.42071
H	0.00784	2.55297	-7.73678
H	-1.49749	3.45057	-7.42097
N	0.01378	4.48952	-8.40937
C	-0.46234	5.72947	-8.64872
C	0.34328	6.20748	-9.65896
N	1.24667	5.24020	-9.94931
N	1.03833	4.22023	-9.18669
H	-1.30200	6.14657	-8.11832
C	0.32897	7.51249	-10.40727
H	-0.07331	7.35988	-11.41064
H	-0.30351	8.22886	-9.88363
C	1.76973	8.04751	-10.51612
H	2.18666	8.28050	-9.53983
H	2.41296	7.33220	-11.01976
C	1.63982	11.57580	-12.79870
C	1.38854	11.63569	-11.42224

C	1.46979	10.45666	-10.70702
N	1.77731	9.29717	-11.31894
C	2.01842	9.23521	-12.63451
C	1.96229	10.37639	-13.42690
H	1.58179	12.48472	-13.38658
H	1.29591	10.40348	-9.64097
H	2.25716	8.26024	-13.03782
C	-0.43208	-2.90230	5.11199
H	-1.30765	-3.38816	4.67283
H	0.46784	-3.45564	4.83185
O	-0.55299	-2.80807	6.51550
C	-0.63544	-4.03935	7.20658
H	-1.53163	-4.59364	6.91696
H	0.24665	-4.65558	7.01698
C	-0.70190	-3.65466	8.68208
H	0.19412	-3.08872	8.94416
H	-1.58527	-3.03695	8.85481
O	-0.77257	-4.85280	9.43183
C	-0.85426	-4.70944	13.57580
C	-0.84943	-5.92642	12.88541
C	-0.82084	-5.97588	11.49580
C	-0.79803	-4.75412	10.79272
C	-0.79839	-3.53433	11.46621
C	-0.82726	-3.51910	12.86369
H	-0.87591	-4.70127	14.65761
H	-0.86360	-6.84953	13.45006
H	-0.77644	-2.59978	10.92365
H	-0.82704	-2.56871	13.38191
C	-0.84708	-7.27874	10.70691
H	-0.18868	-7.14696	9.84780
C	-0.35136	-8.48778	11.51593
H	0.62841	-8.29215	11.95517
H	-1.05168	-8.73705	12.31556
H	-0.27325	-9.35307	10.85558
C	-2.27434	-7.53779	10.17648
H	-2.96237	-7.65469	11.01674
H	-2.60811	-6.70491	9.55770
H	-2.29127	-8.45140	9.57879
C	1.03402	12.94080	-10.73827
H	0.87663	12.78494	-9.67247
H	1.84114	13.66007	-10.87981
H	0.12253	13.34566	-11.17913
C	2.25222	10.27939	-14.91247
H	2.03472	11.23022	-15.39489
H	3.30311	10.03260	-15.06899
H	1.63858	9.49987	-15.36416

H -3.38028 5.45952 -0.64777
H -3.38374 -5.45121 0.65009
H -3.38992 -1.11810 2.11308
H -3.23989 1.12009 -2.14513
H -3.38032 5.37575 1.12241
H -3.37472 -5.38726 -1.12055
H -3.27630 -3.52864 1.91252
H -3.12479 3.53046 -1.92935
C -3.32826 -1.54093 1.12291
C -3.23594 1.54123 -1.15184
C -3.16777 2.89799 -1.05444
C -3.25933 -2.89856 1.03468
C -3.29938 0.71032 0.01609
C -3.30076 -0.71399 -0.04802
H -3.41818 0.92698 2.20148
H -3.27566 -0.93404 -2.23762

D1^{+}⊂**CBPQT**$^{(2+)(\bullet+)}$ at DNP
-3679.96716686284
H 0.06017 -2.85632 -1.29950
C -0.05009 -1.77611 0.52578
C -0.07043 -0.48625 1.12658
C 0.01829 -1.88182 -0.83292
C -0.11836 -0.35301 2.55205
H -0.06173 -2.64768 1.15957
C -0.01712 0.67697 0.33366
C 0.04660 -0.72693 -1.66165
C -0.09357 0.88795 3.13766
H 0.09526 -0.85572 -2.73300
H -0.11889 1.00412 4.21190
C 0.01038 1.95773 0.94836
C 0.02478 0.52049 -1.09347
C -0.02056 2.04370 2.31495
O 0.04127 1.67742 -1.80579
C 0.04361 1.54357 -3.21410
H 0.91574 0.97936 -3.54951
H -0.86328 1.03397 -3.54815
O -0.18625 -1.52692 3.22709
C -0.28062 -1.47757 4.63891
H 0.60460 -1.00498 5.06799
H -1.17217 -0.92515 4.94293
H 0.01800 3.00896 2.80089
H 0.07280 2.84071 0.32481
C 0.07356 2.93953 -3.82351
H 1.05808 3.39350 -3.68447
H -0.68691 3.56669 -3.35324

O	-0.20915	2.75776	-5.19513
C	0.04711	3.88980	-5.99756
H	-0.40887	4.78698	-5.57059
H	1.12256	4.05046	-6.10819
C	-0.57298	3.57536	-7.36451
H	-0.22204	2.60493	-7.70772
H	-1.65931	3.58638	-7.32359
N	-0.12829	4.55123	-8.35300
C	-0.59169	5.79282	-8.60775
C	0.24068	6.26316	-9.59963
N	1.14596	5.29036	-9.86442
N	0.91288	4.27344	-9.10478
H	-1.44134	6.21575	-8.09871
C	0.25029	7.56519	-10.35367
H	-0.14856	7.41472	-11.35874
H	-0.37338	8.29379	-9.83653
C	1.70025	8.07656	-10.45606
H	2.11543	8.30539	-9.47810
H	2.33424	7.34896	-10.95373
C	1.64728	11.59919	-12.75192
C	1.39881	11.66978	-11.37544
C	1.45351	10.49200	-10.65534
N	1.73385	9.32325	-11.26263
C	1.97191	9.25099	-12.57828
C	1.94062	10.38968	-13.37554
H	1.60946	12.50786	-13.34255
H	1.27865	10.44722	-9.58911
H	2.18810	8.26945	-12.97788
C	-0.38203	-2.91976	5.12982
H	-1.25251	-3.40607	4.68130
H	0.52091	-3.47243	4.85877
O	-0.51723	-2.82553	6.53104
C	-0.59445	-4.05892	7.22061
H	-1.48490	-4.61894	6.92437
H	0.29335	-4.66788	7.03443
C	-0.67223	-3.67887	8.69678
H	0.21765	-3.10644	8.96563
H	-1.56168	-3.06926	8.86678
O	-0.73731	-4.88058	9.44130
C	-0.85744	-4.75142	13.58541
C	-0.83761	-5.96610	12.89129
C	-0.79653	-6.01130	11.50175
C	-0.77626	-4.78712	10.80271
C	-0.79199	-3.56952	11.48003
C	-0.83343	-3.55871	12.87717
H	-0.88827	-4.74689	14.66699

H	-0.84989	-6.89081	13.45336
H	-0.77273	-2.63308	10.94072
H	-0.84557	-2.60997	13.39828
C	-0.80832	-7.31288	10.71014
H	-0.14122	-7.17687	9.85839
C	-0.31680	-8.52144	11.52257
H	0.65759	-8.32342	11.97256
H	-1.02478	-8.77451	12.31426
H	-0.22897	-9.38546	10.86177
C	-2.22868	-7.57799	10.16413
H	-2.92508	-7.69944	10.99678
H	-2.55994	-6.74595	9.54282
H	-2.23464	-8.49108	9.56534
C	1.07373	12.98554	-10.69718
H	0.92727	12.84037	-9.62839
H	1.89043	13.69050	-10.85472
H	0.16328	13.40161	-11.12978
C	2.22638	10.27908	-14.86086
H	2.03574	11.23463	-15.34547
H	3.26975	10.00168	-15.01786
H	1.59009	9.51586	-15.30962
H	-3.38868	5.43322	-0.59125
H	-3.39778	-5.43789	0.58415
H	-3.80016	-1.14560	2.06377
H	-3.89636	1.14056	-2.02024
H	-3.38030	5.35740	1.18349
H	-3.37777	-5.34394	-1.18988
H	-3.56895	-3.58677	1.83168
H	-3.64895	3.58214	-1.80572
C	-3.55638	-1.55532	1.09350
C	-3.61746	1.55364	-1.06186
C	-3.49390	2.92627	-0.95977
C	-3.43774	-2.92941	0.98320
C	-3.39617	0.74858	0.06368
C	-3.38417	-0.74833	-0.03600
H	-2.94381	0.84324	2.19113
H	-3.01337	-0.83846	-2.18060
C	-3.13459	1.38614	1.27671
C	-3.15188	-1.38353	-1.25810
N	-3.18494	3.50799	0.21384
N	-3.16988	-3.50727	-0.19969
C	-3.03434	2.76658	1.32071
C	-3.04744	-2.76307	-1.30843
H	-2.81256	3.29385	2.23702
H	-2.85473	-3.28869	-2.23394
C	-2.91048	4.98570	0.27611

C	-2.91048	-4.98570	-0.27611
C	-1.40461	5.19734	0.27973
C	-1.40482	-5.21077	-0.27412
H	-1.24604	5.22080	-1.86384
H	-1.23399	-5.14992	1.87429
H	-1.23357	5.35442	2.42163
H	-1.23643	-5.42663	-2.41178
C	-0.70153	5.21050	-0.92771
C	-0.69937	-5.19357	0.93235
C	-0.70133	5.29754	1.47931
C	-0.70262	-5.35019	-1.47177
C	0.68998	5.21568	-0.92933
C	0.69249	-5.20194	0.93140
C	0.69550	5.30193	1.47629
C	0.69472	-5.35395	-1.47113
H	1.22650	5.22038	-1.87011
H	1.22621	-5.16961	1.87408
H	1.23051	5.35555	2.41715
H	1.22764	-5.42601	-2.41179
C	1.39975	5.20699	0.27644
C	1.40069	-5.22080	-0.27501
C	2.91048	4.98570	0.27611
C	2.91048	-4.98570	-0.27611
H	3.17990	3.31735	2.26524
H	3.22466	-3.32491	-2.26352
N	3.18791	3.53551	0.19834
N	3.17872	-3.53448	-0.19617
C	3.22149	2.77746	1.32976
C	3.23890	-2.78093	-1.32934
H	3.22558	-3.54905	1.88283
H	3.28519	3.55560	-1.87797
H	3.38014	5.46141	-0.58272
H	3.38261	-5.45855	0.58299
C	3.26290	2.91108	-1.01094
C	3.22983	-2.90785	1.01294
H	3.36585	5.36780	1.18704
H	3.36933	-5.36421	-1.18675
C	3.29656	1.41781	1.28603
C	3.31602	-1.42081	-1.28761
H	3.31306	0.89900	2.23169
H	3.36711	-0.90389	-2.23358
C	3.29856	-1.55141	1.12037
C	3.33262	1.55536	-1.12098
C	3.31648	0.71143	0.03897
C	3.31136	-0.71166	-0.04156
H	3.34132	-1.13983	2.11689

H 3.40938 1.14711 -2.11671

D1^{+}⊂**CBPQT**$^{4+}$ at DNP
-3679.82027315527
H 0.05896 -2.68507 -2.24094
C -0.02094 -1.89593 -0.26440
C -0.04544 -0.70581 0.51967
C 0.04198 -1.79718 -1.62672
C -0.13219 -0.75985 1.95141
H -0.05408 -2.85752 0.23071
C 0.00648 0.55941 -0.10344
C 0.07879 -0.53761 -2.28062
C -0.14825 0.39738 2.69017
H 0.11824 -0.51598 -3.35966
H -0.21365 0.37913 3.76800
C -0.00969 1.75254 0.67410
C 0.06261 0.61286 -1.53627
C -0.08037 1.65707 2.03568
O 0.08564 1.86205 -2.07497
C 0.00473 1.91991 -3.49013
H 0.87067 1.43849 -3.94681
H -0.90330 1.42010 -3.83319
O -0.20346 -2.00910 2.48807
C -0.28437 -2.06297 3.90577
H 0.59135 -1.58616 4.34845
H -1.18454 -1.54973 4.24902
H -0.09134 2.54688 2.65009
H 0.03271 2.71143 0.17384
C -0.05733 3.37571 -3.93722
H 0.91802 3.85828 -3.83798
H -0.79760 3.92667 -3.35218
O -0.44947 3.29307 -5.29059
C -0.24454 4.45998 -6.05588
H -0.68447 5.33532 -5.57203
H 0.82194 4.63354 -6.21841
C -0.93864 4.17880 -7.39429
H -0.60480 3.21838 -7.77949
H -2.02049 4.18180 -7.29100
N -0.55979 5.18311 -8.38001
C -1.11908 6.38083 -8.64535
C -0.31218 6.91498 -9.62809
N 0.66881 6.01660 -9.87748
N 0.50806 4.98449 -9.11758
H -2.00647 6.73231 -8.14617
C -0.40343 8.21464 -10.38374
H -1.27785 8.20605 -11.03569

H -0.50434 9.04544 -9.68481
C 0.86410 8.39896 -11.23705
H 1.75569 8.48617 -10.62192
H 0.99536 7.58048 -11.93828
C 0.37401 11.96032 -13.41527
C 0.91872 12.01194 -12.12645
C 1.08794 10.81596 -11.45499
N 0.73841 9.64923 -12.02784
C 0.21895 9.59430 -13.26058
C 0.01825 10.75049 -14.00545
H 0.22697 12.88403 -13.96399
H 1.50109 10.75579 -10.45724
H -0.03003 8.61090 -13.63616
C -0.34125 -3.51138 4.39063
H -1.22636 -4.02129 4.00203
H 0.55896 -4.05751 4.09840
O -0.41729 -3.36353 5.79380
C -0.47524 -4.54511 6.57256
H -1.35985 -5.13648 6.32567
H 0.42043 -5.15379 6.43142
C -0.55553 -4.03613 8.01188
H 0.32246 -3.42135 8.21873
H -1.45696 -3.43094 8.12433
O -0.59402 -5.15416 8.87879
C -0.79893 -4.56004 12.98345
C -0.74273 -5.84433 12.43190
C -0.67241 -6.04712 11.05739
C -0.66096 -4.91083 10.22218
C -0.71143 -3.62517 10.75818
C -0.78138 -3.45585 12.14415
H -0.85186 -4.43400 14.05690
H -0.74978 -6.69908 13.09557
H -0.69673 -2.75469 10.11806
H -0.82034 -2.45436 12.55318
C -0.64493 -7.43341 10.42680
H 0.03869 -7.38806 9.57854
C -0.15193 -8.52698 11.38873
H 0.80997 -8.25967 11.82966
H -0.87148 -8.69629 12.19269
H -0.03738 -9.46221 10.83829
C -2.04885 -7.78813 9.88986
H -2.75987 -7.82283 10.71825
H -2.38084 -7.04177 9.16813
H -2.02733 -8.76573 9.40401
C 1.31267 13.32739 -11.48512
H 1.63852 13.17059 -10.45856

H 2.12574 13.78052 -12.05296
H 0.46010 14.00661 -11.49089
C -0.56185 10.65373 -15.40322
H -0.78965 11.64830 -15.78127
H 0.15651 10.17483 -16.06970
H -1.47466 10.05828 -15.38777
H -3.37532 5.44955 -0.45556
H -3.38493 -5.45746 0.44589
H -3.12655 -1.15959 2.07968
H -2.95573 1.13107 -2.03700
H -3.38958 5.31419 1.31629
H -3.38007 -5.30723 -1.32375
H -2.99008 -3.59140 1.78346
H -2.83640 3.56605 -1.75184
C -3.20065 -1.56221 1.08054
C -3.10130 1.54458 -1.05066
C -3.01534 2.91290 -0.91201
C -3.10815 -2.93161 0.93668
C -3.35331 0.74426 0.07068
C -3.35759 -0.75131 -0.04960
H -3.80663 0.85472 2.19723
H -3.64830 -0.83975 -2.20758
C -3.55608 1.38688 1.29252
C -3.46985 -1.38127 -1.29076
N -3.16127 3.49969 0.28872
N -3.16391 -3.50419 -0.27824
C -3.44309 2.76753 1.37465
C -3.35768 -2.76005 -1.37615
H -3.58318 3.29844 2.30578
H -3.42355 -3.28217 -2.32001
C -2.90715 4.97542 0.40344
C -2.90715 -4.97542 -0.40344
C -1.39993 5.18593 0.43286
C -1.40024 -5.19924 -0.41991
H -1.23819 5.63515 -1.66526
H -1.23279 -5.53466 1.70311
H -1.23136 4.91198 2.56477
H -1.22953 -5.04168 -2.56319
C -0.69900 5.43300 -0.74763
C -0.69740 -5.39435 0.77189
C -0.69673 5.04028 1.63099
C -0.69672 -5.12651 -1.62332
C 0.69633 5.42728 -0.75070
C 0.69732 -5.39778 0.77210
C 0.69619 5.03969 1.62954
C 0.69775 -5.12890 -1.62314

H 1.23193 5.61495 -1.67363
H 1.23163 -5.54288 1.70340
H 1.23191 4.91095 2.56255
H 1.23174 -5.04405 -2.56242
C 1.39849 5.18219 0.42999
C 1.40075 -5.20447 -0.41992
C 2.90715 4.97542 0.40344
C 2.90715 -4.97542 -0.40344
H 3.53430 3.29156 2.31030
H 3.55191 -3.29454 -2.29999
N 3.16537 3.50105 0.28233
N 3.15106 -3.50008 -0.27948
C 3.41808 2.76393 1.37383
C 3.42390 -2.76590 -1.36621
H 2.82270 -3.56855 1.76375
H 2.88740 3.57482 -1.76829
H 3.37605 5.45527 -0.45195
H 3.38856 -5.45142 0.44749
C 3.05050 2.92059 -0.92460
C 3.01029 -2.91739 0.92389
H 3.38558 5.31156 1.31932
H 3.38309 -5.30378 -1.32332
C 3.52714 1.38443 1.29117
C 3.53839 -1.38659 -1.28150
H 3.75274 0.84537 2.19942
H 3.78204 -0.85088 -2.18594
C 3.09981 -1.54831 1.06564
C 3.13973 1.55108 -1.06547
C 3.35404 0.74764 0.06047
C 3.34719 -0.74748 -0.05592
H 2.95225 -1.13683 2.05321
H 3.01734 1.14273 -2.05777

D1^{+}⊂**CBPQT**$^{2(\bullet+)}$ at isopropylphenyl group, relative shift=0
-3680.07269216393
H 1.21829 -2.57134 -12.86999
C 0.73946 -0.89907 -11.64674
C 0.38065 0.48034 -11.62475
C 0.94203 -1.52522 -12.84492
C 0.19503 1.18771 -10.39002
H 0.85200 -1.42945 -10.71241
C 0.22075 1.18968 -12.83183
C 0.79959 -0.82832 -14.07728
C -0.13593 2.51854 -10.38339
H 0.97402 -1.35119 -15.00714
H -0.27467 3.05581 -9.45610

C	-0.12472	2.57275	-12.81330
C	0.43956	0.49399	-14.06683
C	-0.29722	3.20910	-11.61677
O	0.26506	1.25450	-15.17853
C	0.77870	0.78311	-16.41519
H	1.84747	0.57980	-16.32460
H	0.25892	-0.11985	-16.73752
O	0.38371	0.43723	-9.27304
C	0.33434	1.09485	-8.01852
H	1.06290	1.90723	-7.98755
H	-0.66510	1.49209	-7.83247
H	-0.55607	4.25964	-11.59208
H	-0.23754	3.09940	-13.74957
C	0.54677	1.91394	-17.41512
H	0.86533	2.86245	-16.97632
H	-0.51397	1.97544	-17.66946
O	1.32380	1.61201	-18.55927
C	0.96485	2.36366	-19.69851
H	0.03790	1.98153	-20.13443
H	0.83362	3.41923	-19.44749
C	2.11677	2.19313	-20.69822
H	2.99100	2.77105	-20.40995
H	2.37476	1.13986	-20.77707
N	1.68749	2.61279	-22.02906
C	1.61884	3.84872	-22.56757
C	1.04960	3.64255	-23.80551
N	0.81689	2.31324	-23.92798
N	1.19857	1.71253	-22.85232
H	1.96604	4.73017	-22.05487
C	0.70772	4.58297	-24.92785
H	-0.33745	4.44000	-25.20725
H	0.84986	5.61418	-24.60770
C	1.60301	4.25835	-26.14142
H	2.63880	4.53547	-25.96253
H	1.55000	3.20101	-26.38468
C	0.17993	6.43667	-29.44829
C	0.92525	7.08954	-28.45818
C	1.39509	6.32829	-27.40606
N	1.13447	5.00872	-27.33621
C	0.42149	4.38057	-28.27948
C	-0.07927	5.07135	-29.37838
H	-0.20165	7.00986	-30.28583
H	1.98466	6.74338	-26.60058
H	0.26211	3.31971	-28.14082
C	0.68351	0.05774	-6.95416
H	-0.05547	-0.74718	-6.95393

H 1.67289 -0.36231 -7.14985
O 0.66383 0.76398 -5.72947
C 0.92650 -0.01816 -4.58105
H 0.21195 -0.84020 -4.49946
H 1.94042 -0.42562 -4.60549
C 0.76740 0.93446 -3.39848
H 1.45556 1.77463 -3.51643
H -0.25853 1.30988 -3.37487
O 1.04974 0.20588 -2.22105
C -0.17440 1.67824 1.45938
C 0.00522 0.31555 1.25111
C 0.36601 -0.17283 0.00000 #constrained
C 0.59969 0.73195 -1.04265
C 0.36842 2.08158 -0.86527
C -0.02071 2.53992 0.39039
H -0.45681 2.05805 2.43340
H -0.15873 -0.36789 2.07174
H 0.49741 2.77478 -1.68222
H -0.19286 3.58459 0.53293
C 0.41490 -1.64517 -0.30762
H 1.42690 -1.90048 -0.60477
C 0.04751 -2.44473 0.93600
H 0.76317 -2.27340 1.74070
H -0.94219 -2.16070 1.28543
H 0.04009 -3.49427 0.69842
C -0.51731 -1.95680 -1.51069
H -1.08903 -1.07680 -1.80647
H 0.06024 -2.29955 -2.36915
H -1.21972 -2.73251 -1.23250
C 1.20768 8.57647 -28.53047
H 1.76538 8.90213 -27.65412
H 1.78801 8.79641 -29.42699
H 0.26588 9.12392 -28.57921
C -0.86825 4.32844 -30.43965
H -1.25783 5.03247 -31.17220
H -0.22217 3.60976 -30.94506
H -1.69911 3.79093 -29.98238
H -3.40352 5.38623 -0.96170
H -3.33431 -5.46555 0.96103
H -3.27126 -1.02603 2.26499
H -3.39750 0.95855 -2.12548
H -3.40947 5.43958 0.80934
H -3.42105 -5.43738 -0.80501
H -3.02196 -3.43222 2.15578
H -3.14813 3.36610 -2.09417
C -3.35296 -1.49866 1.29708

C -3.35594 1.45017 -1.16477
C -3.20470 2.80876 -1.16998
C -3.21025 -2.85729 1.25908
C -3.42567 0.70257 0.05880
C -3.51316 -0.72734 0.09487
H -3.44680 1.09068 2.22295
H -4.02486 -1.08900 -2.01580
C -3.37303 1.52159 1.23587
C -3.74635 -1.53412 -1.07221
N -3.12976 3.54149 -0.02186
N -3.25853 -3.56671 0.09275
C -3.22987 2.87876 1.16498
C -3.60747 -2.89178 -1.04495
H -3.18774 3.48986 2.05615
H -3.75177 -3.49486 -1.93082
C -2.91554 5.01611 -0.06238
C -2.91554 -5.01611 0.06238
C -1.41765 5.36339 -0.06723
C -1.40836 -5.27808 -0.01331
H -1.17988 5.09248 -2.19455
H -1.18748 -5.89694 2.03868
H -1.27646 5.84722 2.03024
H -1.27083 -4.86173 -2.12460
C -0.67360 5.24166 -1.24786
C -0.67539 -5.66118 1.11306
C -0.72874 5.67052 1.11195
C -0.72035 -5.06840 -1.21381
C 0.72129 5.23381 -1.21486
C 0.72487 -5.66438 1.08249
C 0.67361 5.65280 1.14475
C 0.67206 -5.05234 -1.24067
H 1.27171 5.08647 -2.13772
H 1.27606 -5.90555 1.98382
H 1.18122 5.81955 2.08768
H 1.18395 -4.82515 -2.16862
C 1.41198 5.33659 -0.00122
C 1.40810 -5.27329 -0.07215
C 2.91554 5.01611 0.06238
C 2.91554 -5.01611 -0.06238
H 2.75337 3.36210 2.07107
H 3.68321 -3.46050 -2.06839
N 3.16962 3.54706 0.04445
N 3.24789 -3.56245 -0.03411
C 3.02533 2.81135 1.18134
C 3.58069 -2.87121 -1.16854
H 3.03411 -3.45356 2.03228

H 3.66153 3.50307 -1.97653
H 3.43711 5.43894 -0.79373
H 3.37605 -5.46870 0.81397
C 3.52302 2.88883 -1.09754
C 3.21593 -2.86795 1.14130
H 3.35456 5.41141 0.97608
H 3.38342 -5.42737 -0.95502
C 3.20382 1.45732 1.20845
C 3.75836 -1.51468 -1.17505
H 3.04942 0.96856 2.15789
H 3.99513 -1.05743 -2.12335
C 3.38424 -1.51422 1.19820
C 3.70365 1.53262 -1.13890
C 3.52094 0.71038 0.02488
C 3.57821 -0.72220 0.01333
H 3.33612 -1.06124 2.17650
H 3.97937 1.10449 -2.09078

D1$^{+}\subset$ **CBPQT**$^{(2+)(\bullet+)}$ at isopropylphenyl group, relative shift=0.5
-3679.92403291447
H 1.51540 -2.53770 -12.43145
C 0.94258 -0.92502 -11.16869
C 0.49562 0.42730 -11.11488
C 1.17129 -1.51280 -12.38165
C 0.28584 1.09857 -9.86556
H 1.10159 -1.46485 -10.24660
C 0.27374 1.14879 -12.30405
C 0.96821 -0.80138 -13.59682
C -0.12532 2.40631 -9.82732
H 1.16424 -1.29121 -14.54038
H -0.28014 2.91699 -8.88781
C -0.15526 2.50748 -12.25443
C 0.52110 0.49325 -13.55388
C -0.34782 3.10948 -11.04354
O 0.28206 1.26245 -14.64716
C 0.88913 0.89809 -15.87736
H 1.96572 0.77705 -15.74246
H 0.46193 -0.02585 -16.26866
O 0.53836 0.34191 -8.76633
C 0.47209 0.98664 -7.50802
H 1.16666 1.82809 -7.47765
H -0.54053 1.34115 -7.31271
H -0.66861 4.14187 -10.99339
H -0.31238 3.04357 -13.17873
C 0.61321 2.05690 -16.83198
H 0.83073 3.00406 -16.33251

H -0.43483 2.04645 -17.14039
O 1.46894 1.87500 -17.94437
C 1.09630 2.63564 -19.07240
H 0.21533 2.20177 -19.55278
H 0.88015 3.67096 -18.79720
C 2.29098 2.57593 -20.03353
H 3.10198 3.22443 -19.71323
H 2.64046 1.54926 -20.11092
N 1.86995 2.97488 -21.37268
C 1.79276 4.20223 -21.92875
C 1.23514 3.97231 -23.16765
N 1.01496 2.63927 -23.27247
N 1.39648 2.05799 -22.18635
H 2.12839 5.09370 -21.42607
C 0.89773 4.89075 -24.30914
H -0.15952 4.78319 -24.55758
H 1.09212 5.92466 -24.02763
C 1.74817 4.48626 -25.53051
H 2.79744 4.73213 -25.38864
H 1.65094 3.42257 -25.72751
C 0.32341 6.56897 -28.89615
C 1.13418 7.23147 -27.96562
C 1.60022 6.50157 -26.88958
N 1.27562 5.20256 -26.74369
C 0.49879 4.56584 -27.62870
C -0.00385 5.22493 -28.74569
H -0.05520 7.11736 -29.75140
H 2.23757 6.92467 -26.12518
H 0.29085 3.52313 -27.42943
C 0.86798 -0.03383 -6.44738
H 0.15171 -0.85869 -6.42728
H 1.86652 -0.42757 -6.65253
O 0.84255 0.68932 -5.23387
C 1.05882 -0.07583 -4.07111
H 0.34626 -0.90169 -4.00667
H 2.07520 -0.47812 -4.04334
C 0.83639 0.89293 -2.91433
H 1.53236 1.73001 -2.99965
H -0.18841 1.27050 -2.95855
O 1.04741 0.17461 -1.71672
C -0.28090 1.70140 1.90163
C -0.05830 0.33552 1.72911
C 0.34981 -0.16308 0.50000 #constrained
C 0.58560 0.72537 -0.55909
C 0.32818 2.07091 -0.41564
C -0.10650 2.54783 0.82265

H	-0.60099	2.09038	2.85975
H	-0.21880	-0.33583	2.56145
H	0.47538	2.74729	-1.24114
H	-0.28007	3.59761	0.94308
C	0.43245	-1.63137	0.18737
H	1.42743	-1.83972	-0.19027
C	0.20715	-2.46021	1.44869
H	0.95944	-2.22248	2.20234
H	-0.77091	-2.26198	1.88368
H	0.27160	-3.51213	1.21428
C	-0.56359	-1.93236	-0.96826
H	-1.09386	-1.03194	-1.27888
H	-0.04295	-2.33037	-1.83720
H	-1.28885	-2.66665	-0.64549
C	1.48561	8.69697	-28.12428
H	2.13349	9.02430	-27.31321
H	1.99490	8.85197	-29.07592
H	0.57220	9.29257	-28.11439
C	-0.86636	4.47097	-29.73974
H	-1.23259	5.15387	-30.50369
H	-0.28044	3.68402	-30.21614
H	-1.71517	4.01520	-29.22944
H	-3.39210	5.31946	-1.04580
H	-3.31740	-5.45927	1.02362
H	-2.94691	-0.96949	2.28648
H	-3.04103	0.82524	-1.98694
H	-3.43236	5.45828	0.72410
H	-3.44395	-5.40779	-0.74341
H	-2.75902	-3.42635	2.18173
H	-2.81191	3.26647	-2.04555
C	-3.18600	-1.46961	1.35823
C	-3.16467	1.37766	-1.06657
C	-3.01588	2.75308	-1.11728
C	-3.06400	-2.85273	1.31691
C	-3.46234	0.74292	0.14602
C	-3.54370	-0.76396	0.20403
H	-3.87347	1.16388	2.24105
H	-4.25627	-1.06516	-1.83335
C	-3.61258	1.56142	1.27016
C	-3.89215	-1.52092	-0.92281
N	-3.13600	3.51363	-0.01531
N	-3.27317	-3.53975	0.18104
C	-3.43617	2.93660	1.16065
C	-3.73378	-2.89927	-0.91055
H	-3.54459	3.59108	2.01445
H	-3.94530	-3.50230	-1.78297

C	-2.91548	5.00838	-0.11912
C	-2.91548	-5.00838	0.11912
C	-1.41614	5.33686	-0.11099
C	-1.40846	-5.23343	0.00673
H	-1.13242	4.93974	-2.21578
H	-1.15309	-5.98287	2.01130
H	-1.31864	5.98775	1.94416
H	-1.31369	-4.69171	-2.07892
C	-0.64939	5.13282	-1.26532
C	-0.65926	-5.69243	1.09167
C	-0.75374	5.74230	1.05273
C	-0.74620	-4.95721	-1.19417
C	0.74323	5.12865	-1.20263
C	0.74002	-5.71246	1.02714
C	0.64835	5.72640	1.11446
C	0.64443	-4.95311	-1.24920
H	1.31008	4.92338	-2.10422
H	1.30564	-6.01706	1.89970
H	1.13561	5.96557	2.05221
H	1.13681	-4.68268	-2.17590
C	1.40936	5.31662	0.01394
C	1.40333	-5.25166	-0.11265
C	2.91548	5.00838	0.11912
C	2.91548	-5.00838	-0.11912
H	2.79524	3.35158	2.14582
H	3.51150	-3.39141	-2.11785
N	3.17987	3.54142	0.11205
N	3.25838	-3.55740	-0.05636
C	3.06135	2.80312	1.25301
C	3.49209	-2.83122	-1.19395
H	3.24622	-3.51704	2.02442
H	3.67687	3.50653	-1.90801
H	3.45409	5.43334	-0.72534
H	3.38439	-5.48877	0.73726
C	3.53569	2.88859	-1.03203
C	3.34426	-2.90228	1.13980
H	3.32618	5.41149	1.04220
H	3.36486	-5.40015	-1.02977
C	3.25896	1.45033	1.27727
C	3.68563	-1.47848	-1.17284
H	3.12408	0.95701	2.22729
H	3.85250	-0.99414	-2.12248
C	3.52601	-1.54926	1.22428
C	3.72817	1.53493	-1.07577
C	3.56463	0.70856	0.08690
C	3.61812	-0.72328	0.05010

H 3.57640 -1.12372 2.21622
H 4.02426 1.11542 -2.02550

D1^{+}⊂**CBPQT**$^{4+}$ at isopropylphenyl group, relative shift=0.6
-3679.77848581227
H 3.94006 -1.34028 -12.10130
C 2.47535 -0.66643 -10.71336
C 1.39756 0.23822 -10.48536
C 3.12608 -0.65159 -11.91572
C 0.68450 0.26046 -9.23727
H 2.75907 -1.35700 -9.93261
C 1.00176 1.13566 -11.50078
C 2.75761 0.25549 -12.94807
C -0.37132 1.11571 -9.05084
H 3.29972 0.24058 -13.88299
H -0.92482 1.12950 -8.12322
C -0.08683 2.02982 -11.28502
C 1.71925 1.12769 -12.74557
C -0.75119 2.00834 -10.09193
O 1.28355 2.03336 -13.66126
C 2.07147 2.25082 -14.82511
H 3.08093 2.55505 -14.54195
H 2.11836 1.34743 -15.43447
O 1.14038 -0.61300 -8.29254
C 0.37880 -0.74265 -7.10247
H 0.29739 0.21916 -6.59501
H -0.61997 -1.11493 -7.33660
H -1.58211 2.68009 -9.92011
H -0.37226 2.71097 -12.07342
C 1.39804 3.37570 -15.61428
H 1.17708 4.21640 -14.95290
H 0.46800 3.01449 -16.05916
O 2.32162 3.76000 -16.61937
C 1.75076 4.51119 -17.67299
H 1.07857 3.88552 -18.26433
H 1.19746 5.37207 -17.29132
C 2.92969 4.97380 -18.54661
H 3.44141 5.82836 -18.11331
H 3.62712 4.14802 -18.67011
N 2.46441 5.35679 -19.88135
C 2.44704 6.56091 -20.49255
C 1.92383 6.29767 -21.74110
N 1.66681 4.96816 -21.79771
N 1.99700 4.42139 -20.67697
H 2.79589 7.46122 -20.01606
C 1.63258 7.18102 -22.92698

H 0.55498 7.22015 -23.09666
H 1.99621 8.19073 -22.74172
C 2.31955 6.57596 -24.16880
H 3.40085 6.66993 -24.11308
H 2.05619 5.52816 -24.27813
C 1.00783 8.57803 -27.63112
C 2.07087 9.10965 -26.89110
C 2.48009 8.41460 -25.76827
N 1.87177 7.26895 -25.40605
C 0.85201 6.75934 -26.10989
C 0.38082 7.39413 -27.25374
H 0.66982 9.10022 -28.51944
H 3.29652 8.74265 -25.13945
H 0.42705 5.83382 -25.74479
C 1.08370 -1.73715 -6.17484
H 1.35554 -2.64048 -6.72100
H 1.98368 -1.28723 -5.75326
O 0.13044 -2.03532 -5.16134
C 0.59807 -2.35557 -3.86204
H 0.01189 -3.19186 -3.48508
H 1.65176 -2.63880 -3.88405
C 0.35249 -1.10854 -3.00484
H 1.05650 -0.32900 -3.31231
H -0.65966 -0.76449 -3.22651
O 0.48569 -1.38060 -1.61642
C 0.15062 1.92254 0.92068
C 0.42288 0.65825 1.42135
C 0.52875 -0.45950 0.60000 #constrained
C 0.37185 -0.28663 -0.79034
C 0.09275 0.98367 -1.30006
C -0.02265 2.07754 -0.44628
H 0.06227 2.75813 1.59719
H 0.53003 0.53521 2.49151
H -0.05325 1.14462 -2.35736
H -0.25406 3.04046 -0.86990
C 0.57096 -1.81035 1.29166
H 1.00118 -2.55321 0.62125
C 1.29883 -1.80587 2.65287
H 2.20759 -1.20871 2.64502
H 0.64469 -1.41326 3.43258
H 1.55418 -2.83024 2.93074
C -0.90319 -2.16284 1.55290
H -1.37182 -1.33154 2.08276
H -1.40053 -2.30461 0.59592
H -0.99997 -3.05929 2.16304
C 2.74879 10.40057 -27.30492

H	3.59579	10.61480	-26.65594
H	3.09735	10.31667	-28.33459
H	2.03438	11.22237	-27.24369
C	-0.76449	6.78456	-28.03967
H	-1.04612	7.44496	-28.85752
H	-0.46133	5.82040	-28.44911
H	-1.62597	6.63352	-27.38907
H	-3.42189	5.39879	-0.80669
H	-3.37598	-5.39471	0.83362
H	-4.41424	-1.09339	1.94280
H	-4.08414	1.09490	-2.12965
H	-3.37066	5.35161	0.96845
H	-3.35514	-5.42831	-0.94048
H	-4.02994	-3.53110	1.86350
H	-3.67335	3.51896	-1.99396
C	-4.03250	-1.53252	1.03147
C	-3.78196	1.51882	-1.18242
C	-3.56781	2.88589	-1.12418
C	-3.83521	-2.90892	1.00129
C	-3.61748	0.73874	-0.03249
C	-3.68497	-0.76159	-0.07911
H	-3.14898	0.86317	2.08880
H	-3.08181	-0.91678	-2.16434
C	-3.28941	1.39331	1.15746
C	-3.29587	-1.43826	-1.24271
N	-3.22139	3.48404	0.02900
N	-3.34532	-3.51390	-0.09182
C	-3.10344	2.76655	1.15788
C	-3.14209	-2.80963	-1.22081
H	-2.85439	3.30674	2.05993
H	-2.83708	-3.36438	-2.09420
C	-2.92683	4.96161	0.05579
C	-2.92683	-4.96161	-0.05579
C	-1.41069	5.18399	0.02205
C	-1.40468	-5.08851	-0.03607
H	-1.27008	5.41395	-2.11972
H	-1.26741	-5.36494	2.09575
H	-1.18145	5.15724	2.16855
H	-1.18314	-5.04473	-2.18269
C	-0.72225	5.33075	-1.18849
C	-0.71860	-5.24785	1.16850
C	-0.67537	5.17788	1.21036
C	-0.67249	-5.04729	-1.22703
C	0.67561	5.31830	-1.21552
C	0.67774	-5.23360	1.19754
C	0.72061	5.16745	1.18262

C 0.72030 -5.05153 -1.20132
H 1.18723 5.39901 -2.16715
H 1.19066 -5.33599 2.14632
H 1.26412 5.13401 2.11967
H 1.26389 -5.05769 -2.13839
C 1.40820 5.16207 -0.03291
C 1.40683 -5.08432 0.01720
C 2.92683 4.96161 -0.05579
C 2.92683 -4.96161 0.05579
H 3.23386 3.38595 2.00074
H 2.86328 -3.42672 -2.02643
N 3.26738 3.49611 -0.06785
N 3.34731 -3.51165 -0.02172
C 3.35232 2.81930 1.08832
C 3.17403 -2.84330 -1.17419
H 4.04240 -3.47110 1.93037
H 3.40555 3.45913 -2.13613
H 3.37570 5.39621 -0.94491
H 3.33831 -5.35468 0.98103
C 3.44845 2.85883 -1.23802
C 3.84851 -2.87549 1.04953
H 3.39734 5.38380 0.82857
H 3.39299 -5.46128 -0.79092
C 3.56621 1.44944 1.10347
C 3.36486 -1.47714 -1.24676
H 3.58948 0.96213 2.06734
H 3.17122 -0.99156 -2.19096
C 4.08026 -1.50630 1.02658
C 3.68021 1.49511 -1.28195
C 3.70289 0.74728 -0.09775
C 3.75003 -0.75961 -0.10844
H 4.49155 -1.05212 1.91743
H 3.84520 1.04969 -2.25207

D1$^{+}\subset$ **CBPQT**$^{2(\bullet+)}$ at dimethylpyridinium group, relative shift=2.5
-3680.07760573777
H 1.76180 0.54452 18.83246
C 0.96306 2.49349 19.12695
C 0.36422 3.62772 18.50500
C 1.30510 1.40910 18.36859
C 0.01541 4.79781 19.25916
H 1.14160 2.51024 20.19212
C 0.11630 3.62661 17.11774
C 1.07702 1.38746 16.96405
C -0.55366 5.88474 18.64593
H 1.36401 0.51570 16.39303

H -0.81763 6.76889 19.20810
C -0.47835 4.76087 16.49175
C 0.49390 2.46977 16.35826
C -0.80158 5.85354 17.24566
O 0.22971 2.55909 15.02820
C 0.77444 1.57641 14.16238
H 1.85832 1.52553 14.28128
H 0.33696 0.59697 14.36054
O 0.30271 4.72662 20.58466
C 0.09177 5.89017 21.36794
H 0.65687 6.72878 20.95697
H -0.96923 6.14380 21.39876
H -1.25237 6.72089 16.78117
H -0.66096 4.73983 15.42739
C 0.42761 2.03097 12.74710
H 0.75958 3.06107 12.59831
H -0.65278 1.97623 12.59339
O 1.10519 1.15514 11.86386
C 0.72483 1.31712 10.51640
H -0.31638 1.01856 10.37046
H 0.84755 2.35434 10.19317
C 1.64597 0.39753 9.70342
H 2.66868 0.76526 9.70105
H 1.61266 -0.61240 10.10477
N 1.18150 0.33638 8.31699
C 1.64676 0.97529 7.22495
C 0.79319 0.58079 6.21780
N -0.11814 -0.25806 6.76235
N 0.13264 -0.39511 8.02097
H 2.50292 1.62713 7.25436
C 0.73680 0.93416 4.75451
H -0.12871 1.57352 4.60023
H 1.64010 1.47317 4.47540
C 0.59603 -0.37061 3.96666
H 1.50370 -0.96143 4.06822
H -0.24218 -0.94161 4.35808
C -0.04253 -0.01549 -0.19415
C 0.06721 1.13732 0.56279
C 0.27741 1.01226 1.92495
N 0.35446 -0.19674 2.50000 #constrained
C 0.23253 -1.32064 1.76950
C 0.04177 -1.26293 0.40165
H -0.19091 0.05739 -1.26662
H 0.39598 1.87394 2.56171
H 0.30004 -2.25523 2.31191
C 0.59148 5.59079 22.77958

H	0.00923	4.78224	23.22757
H	1.64511	5.30333	22.75108
O	0.41440	6.80051	23.48920
C	0.81552	6.77569	24.84536
H	0.20606	6.07639	25.42290
H	1.86799	6.49753	24.93767
C	0.60104	8.20312	25.34279
H	1.21660	8.88530	24.75354
H	-0.45104	8.47034	25.22773
O	0.97906	8.24122	26.70671
C	0.66096	11.77178	28.86092
C	1.12149	10.59120	29.45435
C	1.22906	9.40631	28.73406
C	0.85691	9.42495	27.37370
C	0.39978	10.59362	26.76848
C	0.30311	11.76790	27.52058
H	0.58891	12.67882	29.44643
H	1.40319	10.60527	30.49912
H	0.12006	10.60532	25.72458
H	-0.05301	12.67211	27.04398
C	1.69132	8.09431	29.35567
H	2.31783	7.59172	28.61810
C	2.51486	8.28815	30.63923
H	3.34733	8.97416	30.47337
H	1.89393	8.67841	31.44852
H	2.91383	7.32350	30.95725
C	0.46998	7.19117	29.63548
H	-0.18904	7.67834	30.35756
H	-0.08488	7.00528	28.71606
H	0.79843	6.23577	30.04954
C	-0.00854	2.45887	-0.12832
H	0.00362	3.28005	0.57907
H	0.83594	2.54131	-0.81078
H	-0.91975	2.49023	-0.72316
C	-0.04824	-2.48917	-0.44880
H	-0.95385	-2.44602	-1.05169
H	0.80499	-2.51349	-1.12609
H	-0.05331	-3.37385	0.17416
H	-3.40171	5.44043	-0.88085
H	-3.38527	-5.44151	0.88959
H	-3.11535	-1.02903	2.18492
H	-3.62889	1.04855	-2.14013
H	-3.38122	5.44342	0.89031
H	-3.40381	-5.43421	-0.88200
H	-2.94992	-3.44140	2.07274
H	-3.46624	3.46034	-2.05346

C -3.16504 -1.49318 1.21074
C -3.46066 1.50584 -1.17651
C -3.37481 2.87072 -1.15188
C -3.07380 -2.85591 1.17204
C -3.32959 0.71765 0.01681
C -3.33165 -0.71439 0.01620
H -3.15450 1.03943 2.19206
H -3.67340 -1.05076 -2.13447
C -3.18349 1.49873 1.21364
C -3.48618 -1.50568 -1.17295
N -3.16014 3.56143 0.00198
N -3.15411 -3.56011 0.00746
C -3.09653 2.86133 1.16897
C -3.39630 -2.87126 -1.14426
H -2.98996 3.45876 2.06016
H -3.50250 -3.46332 -2.04286
C -2.91218 5.03045 -0.00012
C -2.91218 -5.03045 0.00012
C -1.40814 5.31306 -0.01875
C -1.41088 -5.33009 -0.01371
H -1.22658 5.10735 -2.15863
H -1.23144 -5.50853 2.13127
H -1.23248 5.70291 2.09449
H -1.22932 -5.34380 -2.16390
C -0.69657 5.22550 -1.21996
C -0.69991 -5.44565 1.18760
C -0.70022 5.55021 1.16263
C -0.69939 -5.37159 -1.21803
C 0.69675 5.22627 -1.22089
C 0.69909 -5.43667 1.18808
C 0.70031 5.54626 1.16266
C 0.69718 -5.36906 -1.21778
H 1.22548 5.11211 -2.16101
H 1.23133 -5.49202 2.13225
H 1.23342 5.69668 2.09466
H 1.22661 -5.34473 -2.16409
C 1.40842 5.30850 -0.01898
C 1.40909 -5.31950 -0.01279
C 2.91218 5.03045 0.00012
C 2.91218 -5.03045 -0.00012
H 3.19311 3.45759 2.07841
H 3.30467 -3.45164 -2.07181
N 3.18180 3.56406 0.00385
N 3.17246 -3.56142 0.00362
C 3.23743 2.86684 1.17350
C 3.30439 -2.86584 -1.16251

H 3.21774 -3.45551 2.07965
H 3.33566 3.45543 -2.06999
H 3.39840 5.44217 -0.88188
H 3.38444 -5.44488 0.88830
C 3.32273 2.86938 -1.16155
C 3.24848 -2.86572 1.17347
H 3.37990 5.44869 0.88900
H 3.39765 -5.43943 -0.88359
C 3.36535 1.50581 1.20840
C 3.42178 -1.50324 -1.19319
H 3.43736 1.04624 2.18322
H 3.51837 -1.04816 -2.16692
C 3.38051 -1.50477 1.20850
C 3.43165 1.50626 -1.19189
C 3.41415 0.71774 0.00812
C 3.41429 -0.71574 0.00827
H 3.47143 -1.05029 2.18438
H 3.53237 1.05204 -2.16512

D1$^{+}\subset$ **CBPQT**$^{(2+)(\bullet+)}$ at dimethylpyridinium group, relative shift=2.0
-3679.90989550910
H 1.83541 0.76261 18.31262
C 1.01193 2.69909 18.61996
C 0.39859 3.82969 18.00542
C 1.36795 1.62437 17.85436
C 0.03451 4.98988 18.76836
H 1.18974 2.71105 19.68537
C 0.15094 3.83457 16.61769
C 1.14044 1.60937 16.44961
C -0.54960 6.07298 18.16233
H 1.43932 0.74506 15.87338
H -0.82577 6.94967 18.73035
C -0.45930 4.96512 16.00012
C 0.54389 2.68779 15.85010
C -0.79755 6.04774 16.76200
O 0.27969 2.78177 14.51964
C 0.82937 1.80478 13.64986
H 1.91372 1.76052 13.76731
H 0.39814 0.82216 13.84641
O 0.32313 4.91435 20.09347
C 0.10021 6.07168 20.88327
H 0.65365 6.91887 20.47423
H -0.96378 6.31181 20.91828
H -1.26083 6.91180 16.30379
H -0.64189 4.94954 14.93565
C 0.47959 2.25984 12.23462

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C	2.92166	-4.97179	0.20998
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H	3.47577	-0.85165	2.13673
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