

## Supporting Information

### Remote control of anion binding by CH-based receptors

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## Table of contents

1. General information .....	3
2. Synthesis.....	3
3. NMR titrations .....	11
3.1 Titrations of <b>4</b> with But <sub>4</sub> NX in various solvents .....	11
3.2 Titrations of <b>5</b> with But <sub>4</sub> NX in various solvents .....	13
3.3 Titrations of <b>6</b> with But <sub>4</sub> NX in various solvents .....	14
3.4 Titrations of <b>8</b> with But <sub>4</sub> NX in various solvents .....	19
3.5 Titrations of <b>9</b> with But <sub>4</sub> NX in various solvents .....	24
4. Comparison of Cl <sup>-</sup> and Br <sup>-</sup> complexation by receptor <b>6</b> and VT NMR spectra .....	30
5. Theoretical calculations.....	31
6. References .....	75

## 1. General information

All solvents and chemicals used were purchased from Sigma Aldrich, TCI Europe N. V., Roth, Chem Impex Inc. and Euriso-top, were of reagent grade and were used without further purification.

$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra were recorded on Bruker 400 MHz and Varian 600 MHz or 500 MHz instruments with residual solvent signal as internal standard. All 2D NMR spectra were recorded at 298 K on Varian 600 MHz with residual solvent signal as internal standard.

IR spectra were measured on JASCO FT/IR-6200.

High resolution ESI mass spectra were recorded on a SYNAPT spectrometer.

## 2. Synthesis

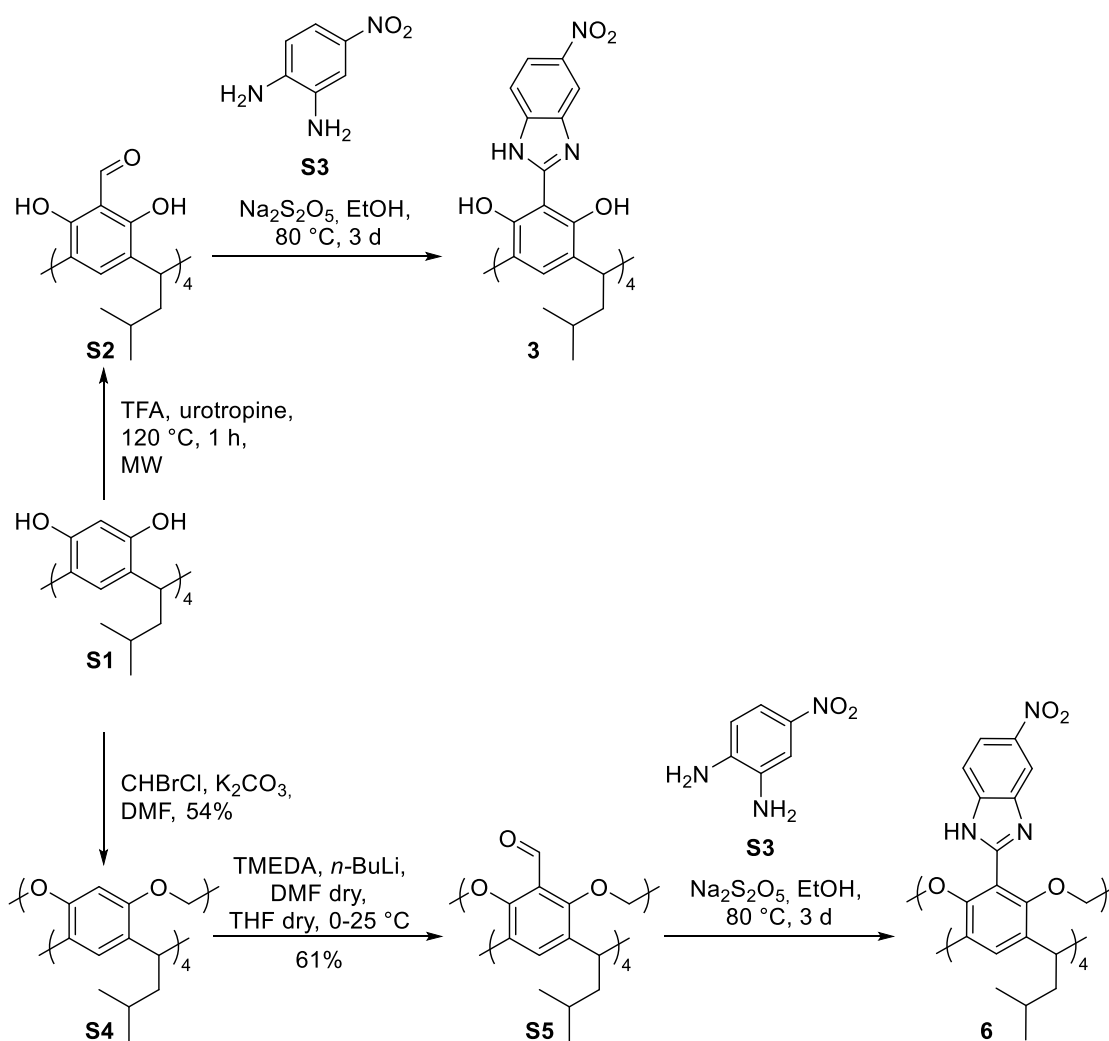


Figure S1. Synthesis of 6 and 9.

**S1:** Obtained by the literature procedure.<sup>1</sup> Analytical data are in agreement with the literature data.  
**S2:** Obtained by the literature procedure.<sup>2</sup> Analytical data are in agreement with the literature data.  
**S4:** Obtained by the literature procedure.<sup>3</sup> Analytical data are in agreement with the literature data.  
**S5:** Obtained by the literature procedure.<sup>3</sup> Analytical data are in agreement with the literature data.  
**4:** Obtained by the literature procedure.<sup>3</sup> Analytical data are in agreement with the literature data.  
**5:** Obtained by the literature procedure.<sup>4</sup> Analytical data are in agreement with the literature data.

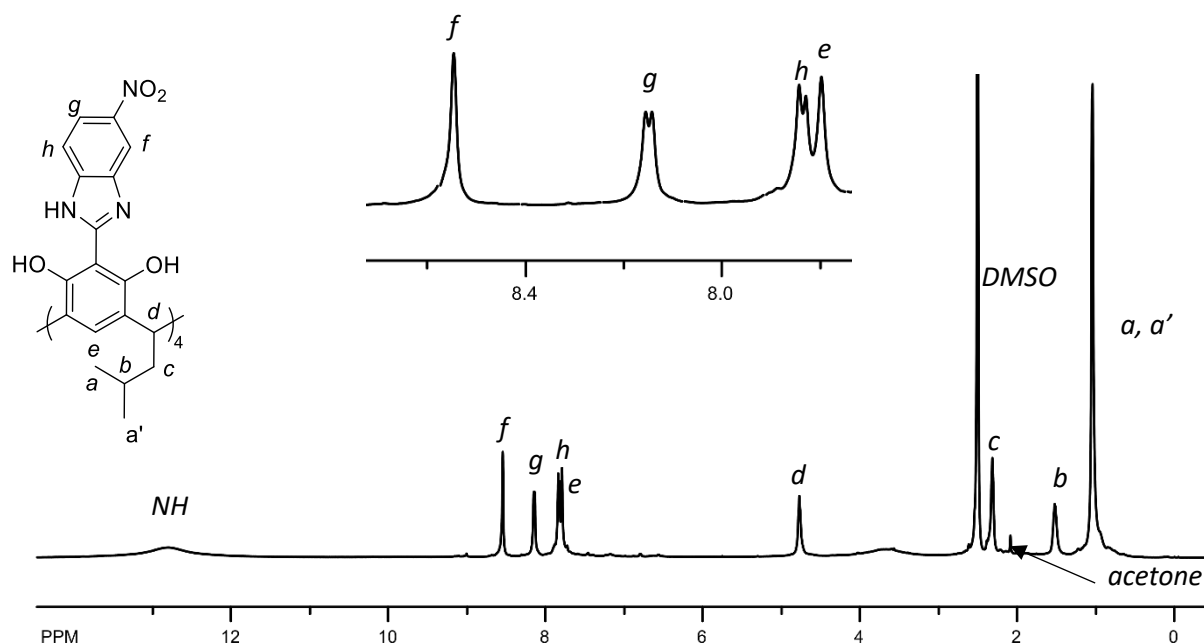
**6:** Tetraformylresorcin[4]arene **S2** (100 mg, 0.106 mmol) and 1,2-diamino-4-nitrobenzene **S3** (65.24 mg, 0.426 mmol) were dissolved in ethanol (5 ml), then 2.85 M solution of Na<sub>2</sub>S<sub>2</sub>O<sub>5</sub> (0.34 ml) was added. The reaction mixture was stirred for 3 days at 80 °C. Then 1 M solution of HCl (2.12 ml) was added. The precipitate was collected and washed with water and diethyl ether. Product **3** was obtained as orange solid, yield 64% (92 mg, 0.0678 mmol).

<sup>1</sup>H NMR (600 MHz, [D<sub>6</sub>]DMSO, 298 K) δ 12.80 (brs, NH), 8.55 (s, 4H), 8.14 (d, *J* = 8.2 Hz, 4H), 7.83 (d, *J* = 8.7 Hz, 4H), 7.79 (s, 4H), 4.77 (brt, 4H), 2.31 (brt, 8H), 1.52 (brm, 4H), 1.04 (d, *J* = 4.9 Hz, 24H).

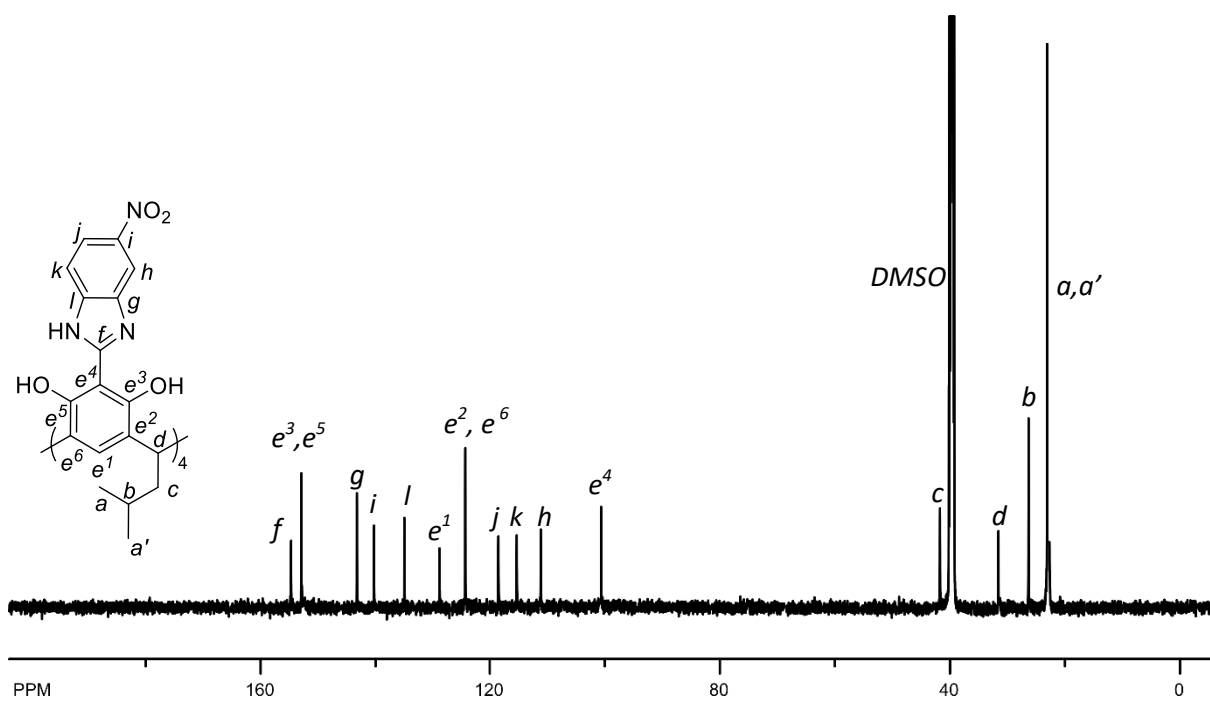
<sup>13</sup>C NMR (150 MHz, [D<sub>6</sub>]DMSO, 298 K) δ 154.5, 152.6, 143.1, 139.9, 134.7, 128.6, 124.3, 118.5, 115.1, 111.1, 100.7, 41.7, 31.3, 26.2, 22.7.

Diffusion coefficient (DOSY) 1.16·10<sup>-10</sup> m<sup>2</sup> s<sup>-1</sup> in [D<sub>6</sub>]DMSO, diameter 1.72 nm.

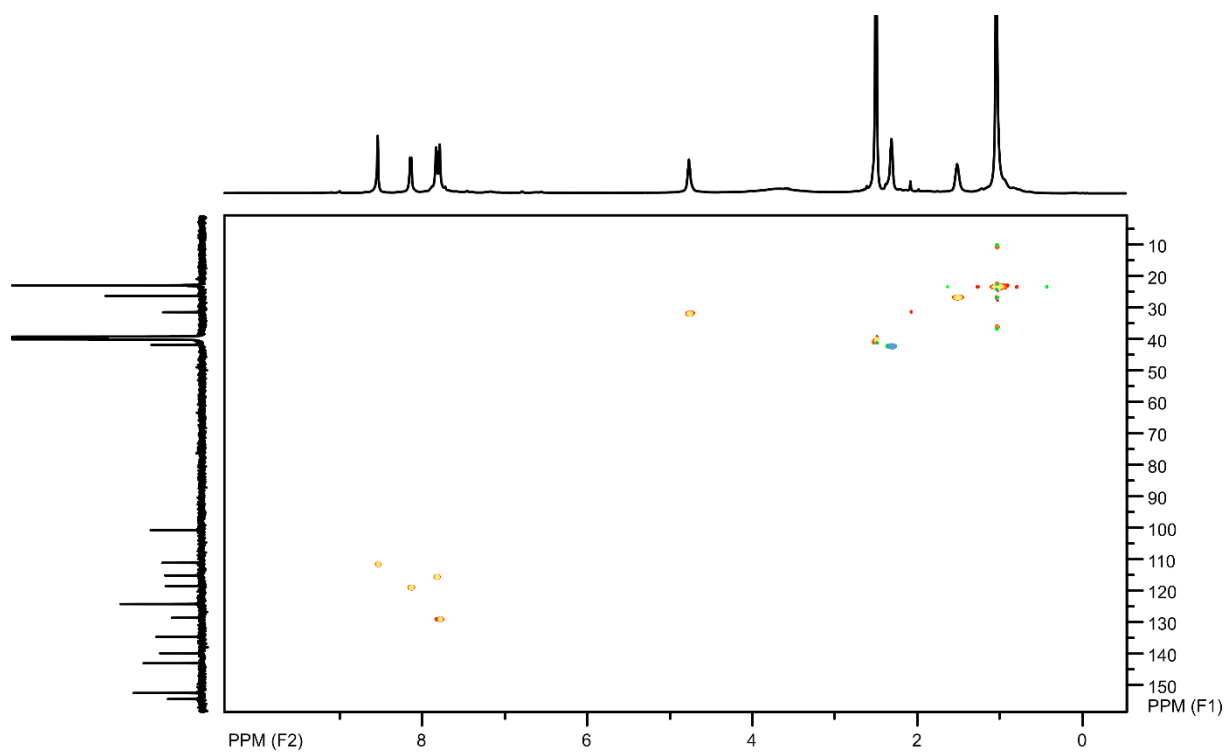
HRMS (ESI): *m/z* calcd for C<sub>72</sub>H<sub>68</sub>N<sub>12</sub>O<sub>16</sub>+Na 1379.4774 [*M* + Na]<sup>+</sup>, found 1379.4783; |Δ| = 0.7 ppm.



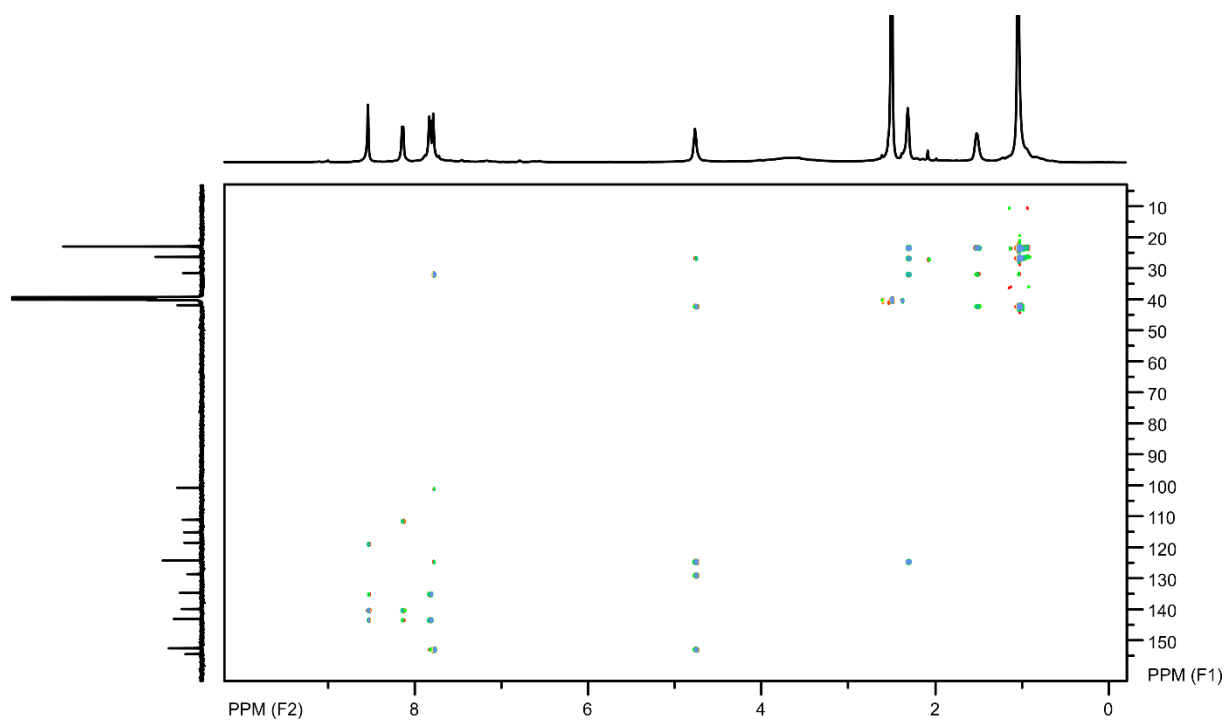
**Figure S2.** <sup>1</sup>H NMR spectrum of **6** (600 MHz, [D<sub>6</sub>]DMSO, 298 K).



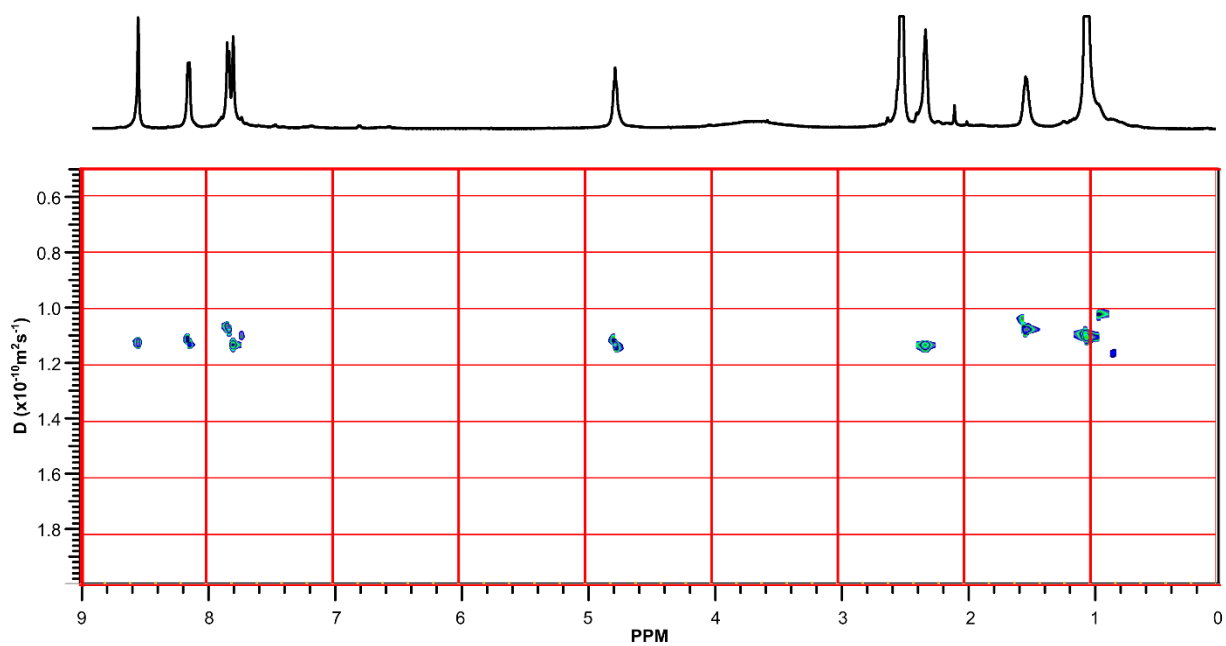
**Figure S3.** <sup>13</sup>C NMR spectrum of **6** (150 MHz, [D<sub>6</sub>]DMSO, 298 K).



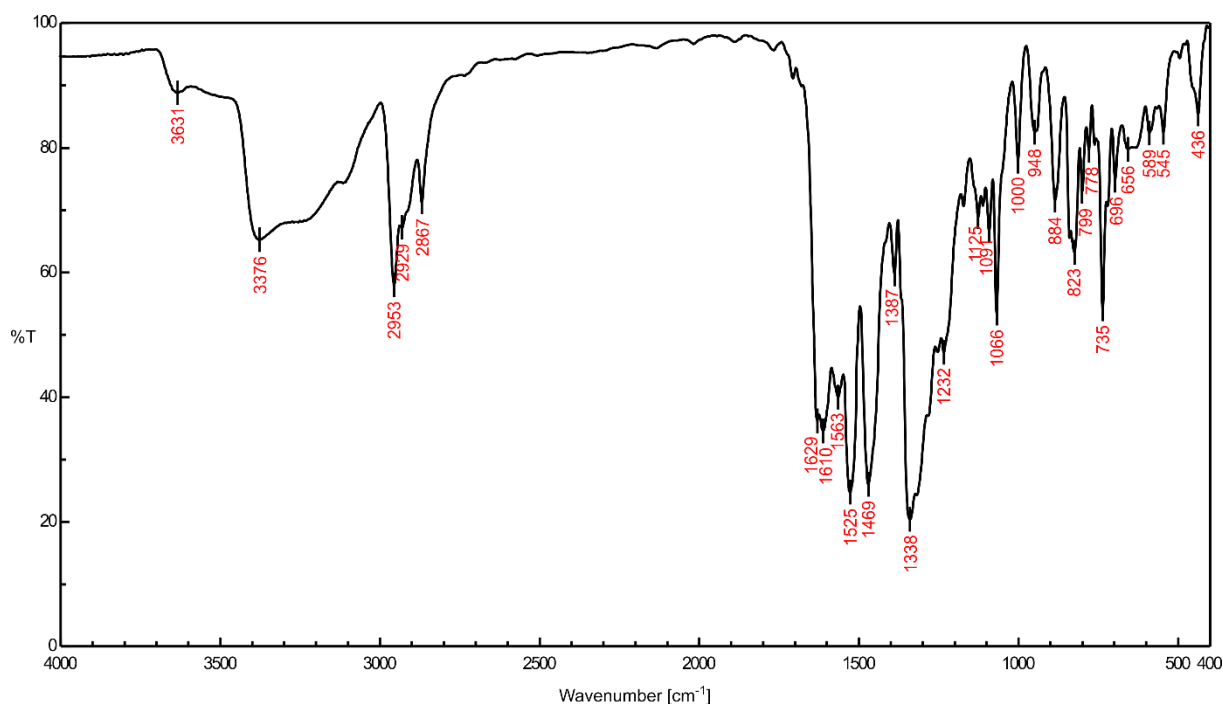
**Figure S4.** HSQC-NMR spectrum of **6** (600 MHz, [D<sub>6</sub>]DMSO, 298 K).



**Figure S5.** HMBC-NMR spectrum of **6** (600 MHz, [D<sub>6</sub>]DMSO, 298 K).



**Figure S6.** DOSY-NMR spectrum of **6** (600 MHz, [D<sub>6</sub>]DMSO, 298 K).



**Figure S7.** FT-IR (KBr) spectrum of **6**.

**7:** Obtained by the literature procedure.<sup>3</sup> Analytical data are in agreement with the literature data.

**8:** Obtained by the literature procedure.<sup>4</sup> Analytical data are in agreement with the literature data.

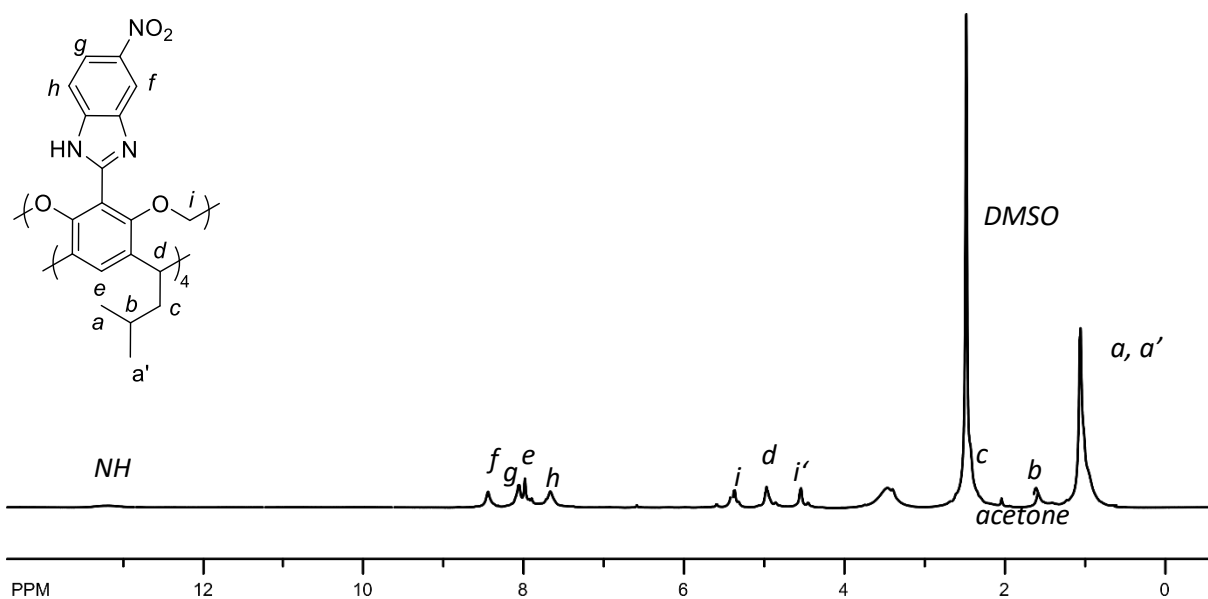
**9:** Tetraformylresorcin[4]arene **S5** (95.54 mg, 0.106 mmol) and 1,2-diamino-4-nitrobenzene **S3** (65.24 mg, 0.426 mmol) were dissolved in ethanol (5 ml), then 2.85 M solution of Na<sub>2</sub>S<sub>2</sub>O<sub>5</sub> (0.34 ml) was added. The reaction mixture was stirred for 3 days at 80 °C. Then 1 M solution of HCl (2.12 ml) was added. The precipitate was collected and washed with water and diethyl ether. Product **9** was obtained as orange solid, yield 60% (89.4 mg, 0.0636 mmol).

<sup>1</sup>H NMR (600 MHz, [D<sub>6</sub>]DMSO, 298 K) δ (broad spectrum) 8.43 (s, 4H), 8.07 (brd, 4H), 8.00 (s, 4H), 7.70 (brd, 4H), 5.37 (brd, 4H), 4.9764 (brt, 4H), 4.56 (brd, 4H), 2.45 (overlap with DMSO, 8H), 1.61 (brm, 4H), 1.07 (brd, 24H).

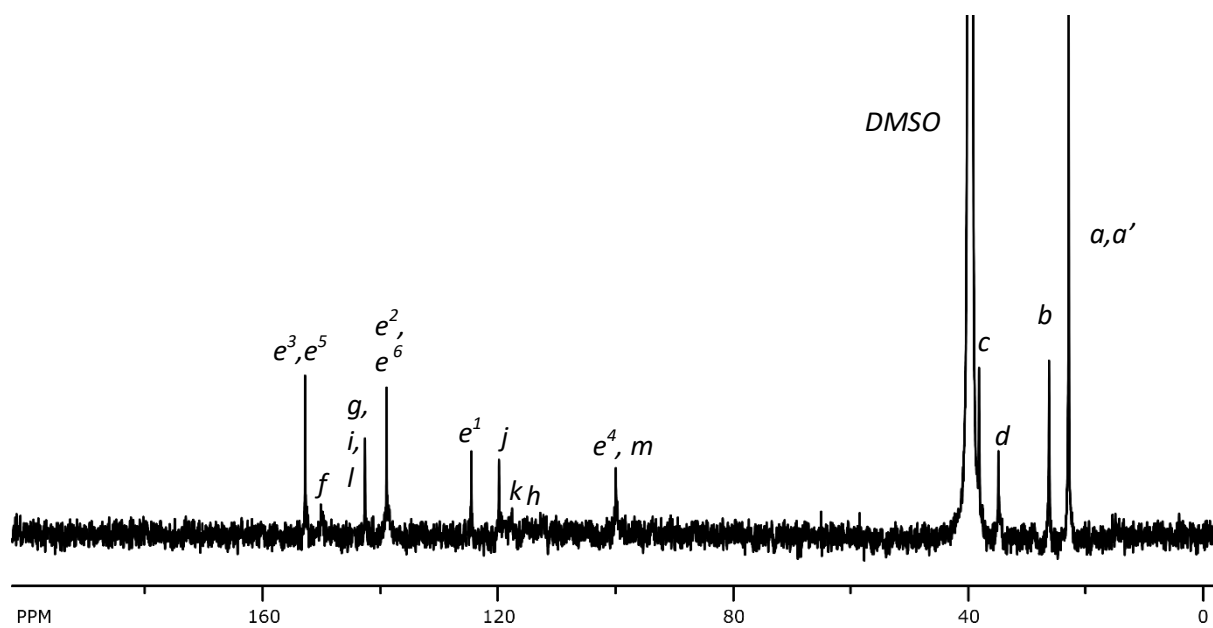
<sup>13</sup>C NMR (150 MHz, [D<sub>6</sub>]DMSO, 298 K) δ 152.6, 149.9, 142.6, 138.7, 124.6, 119.5, 117.7, 113.6, 99.7, 38.0, 34.6, 26.1, 22.6.

**Diffusion coefficient (DOSY)** 1.12·10<sup>-10</sup> m<sup>2</sup> s<sup>-1</sup> in [D<sub>6</sub>]DMSO, diameter **1.78 nm**.

**HRMS (ESI):** m/z calcd for C<sub>72</sub>H<sub>68</sub>N<sub>12</sub>O<sub>16</sub>+Na 1405.4954 [M + H]<sup>+</sup>, found 1405.4938; |Δ| = 1.1 ppm.

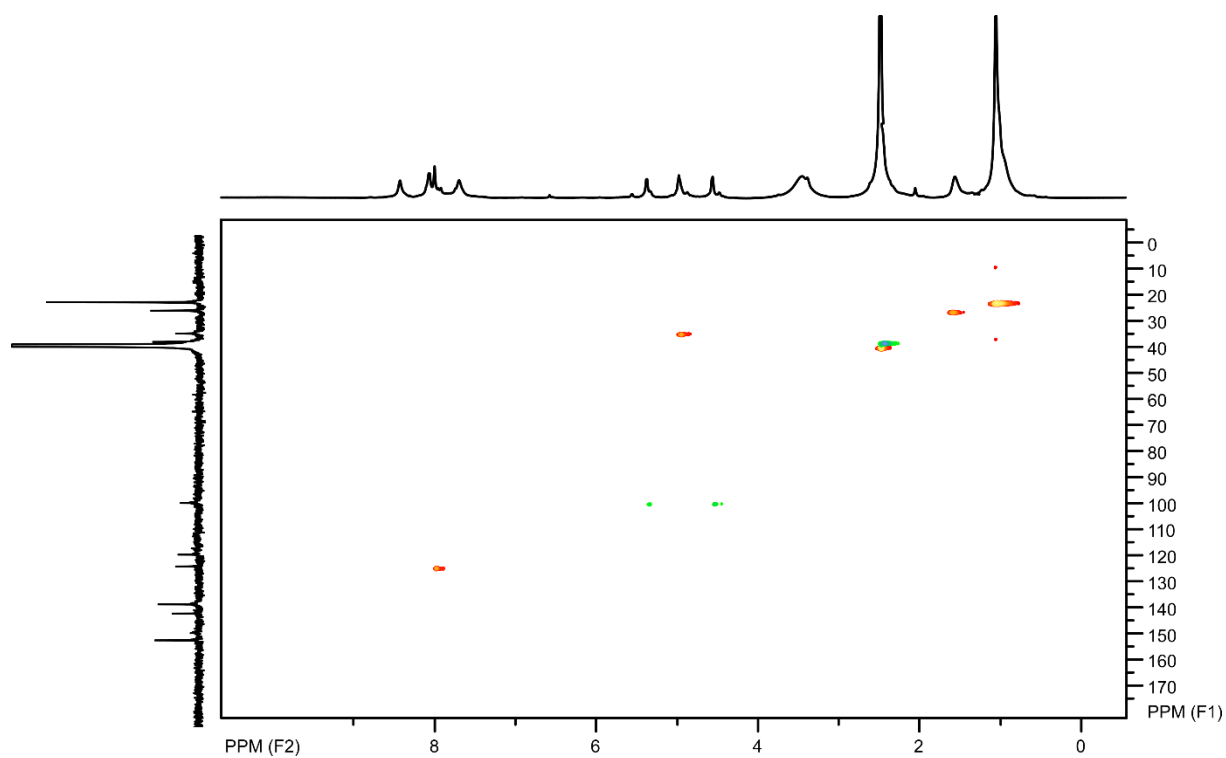


**Figure S8.**  $^1\text{H}$  NMR spectrum of **9** (600 MHz,  $[\text{D}_6]$ DMSO, 298 K).

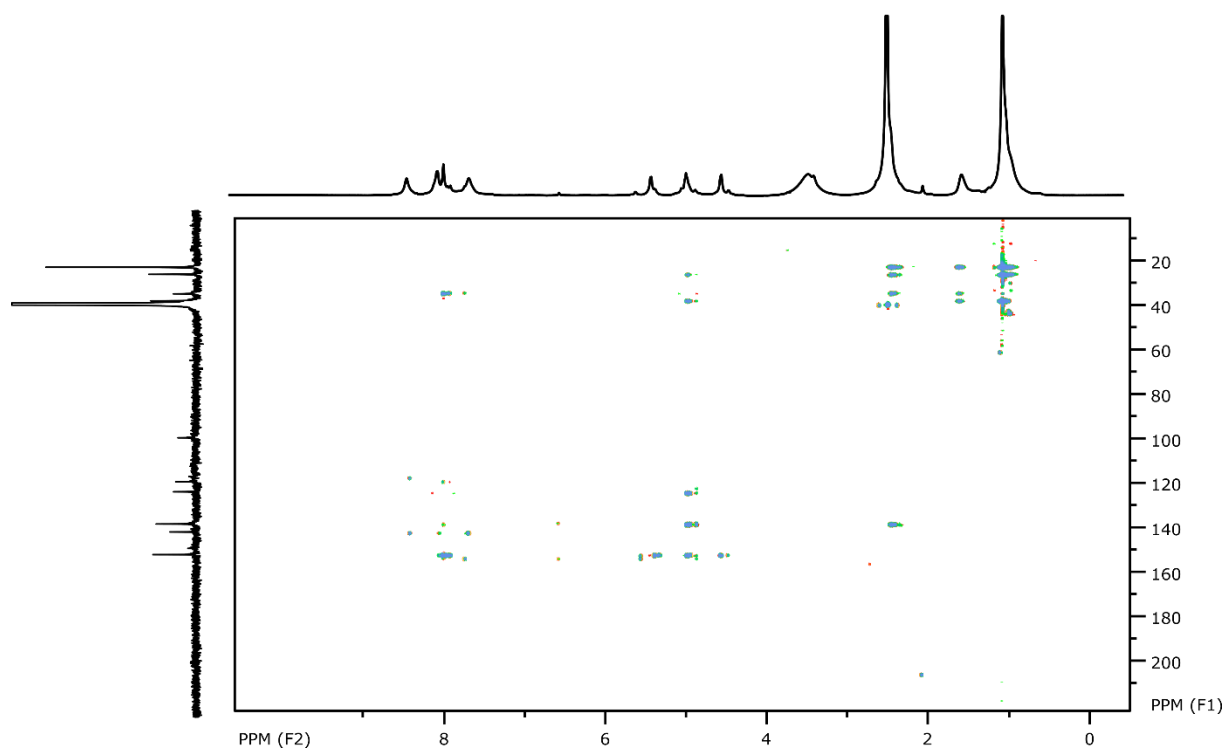


**Figure S9.**  $^{13}\text{C}$  NMR spectrum of **9** (150 MHz,  $[\text{D}_6]$ DMSO, 298 K).

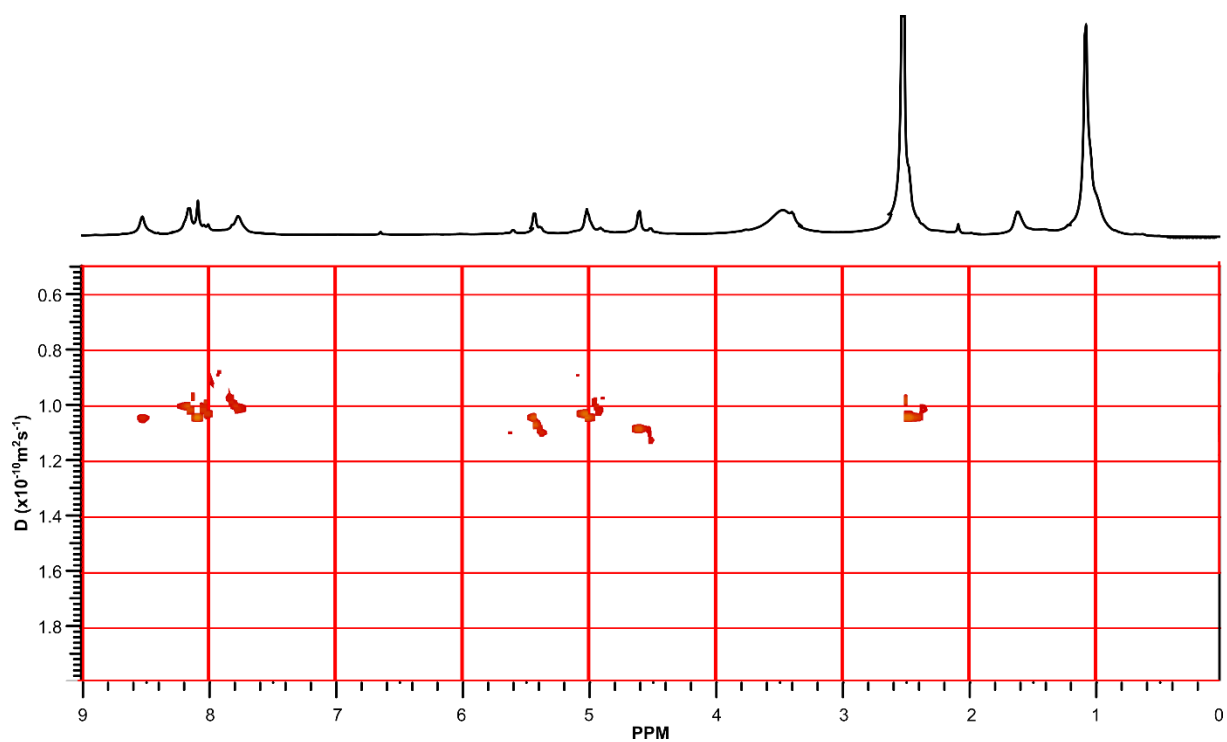




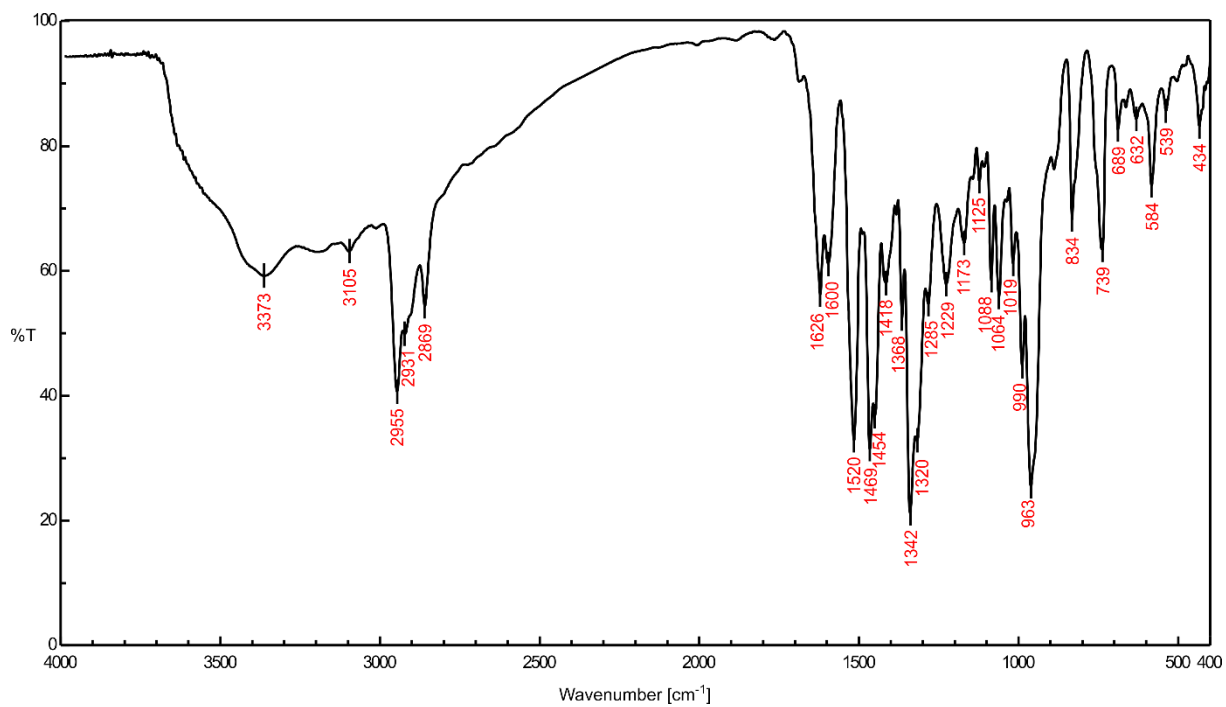
**Figure S10.** HSQC-NMR spectrum of **9** (600 MHz, [D<sub>6</sub>]DMSO, 298 K).



**Figure S11.** HMBC-NMR spectrum of **9** (600 MHz, [D<sub>6</sub>]DMSO, 298 K).



**Figure S12.** DOSY-NMR spectrum of **9** (600 MHz, [D<sub>6</sub>]DMSO, 298 K).



**Figure S13.** FT-IR (KBr) spectrum of **9**.

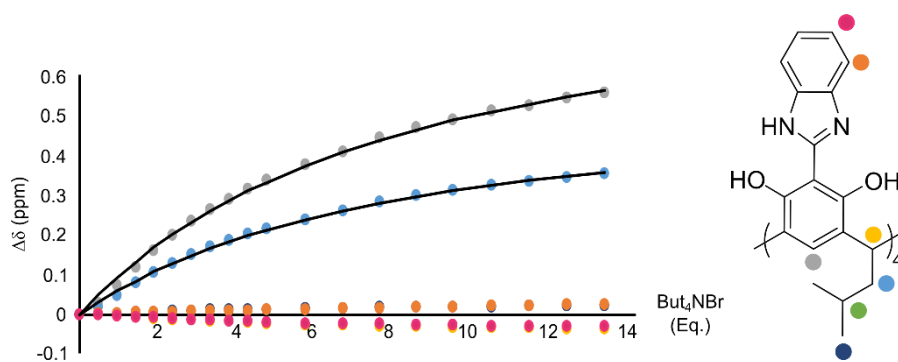
### 3. NMR titrations

#### General procedure for $^1\text{H}$ NMR titrations

To the solution of macrocycle (4-9) ( $C = 2 \text{ mM}$ ) in deuterated solvent:  $[\text{D}_8]\text{THF}$  or  $[\text{D}_6]\text{DMSO}$  or  $[\text{D}_7]\text{DMF}$  or mixture (0.5 ml) a solution containing a guest ( $C = 45 \text{ mM}$ ) and the macrocycle ( $C = 2 \text{ mM}$ ) in deuterated solvent (1 ml) was added in portions.

#### 3.1 Titrations of 4 with $\text{But}_4\text{NBr}$ in various solvents

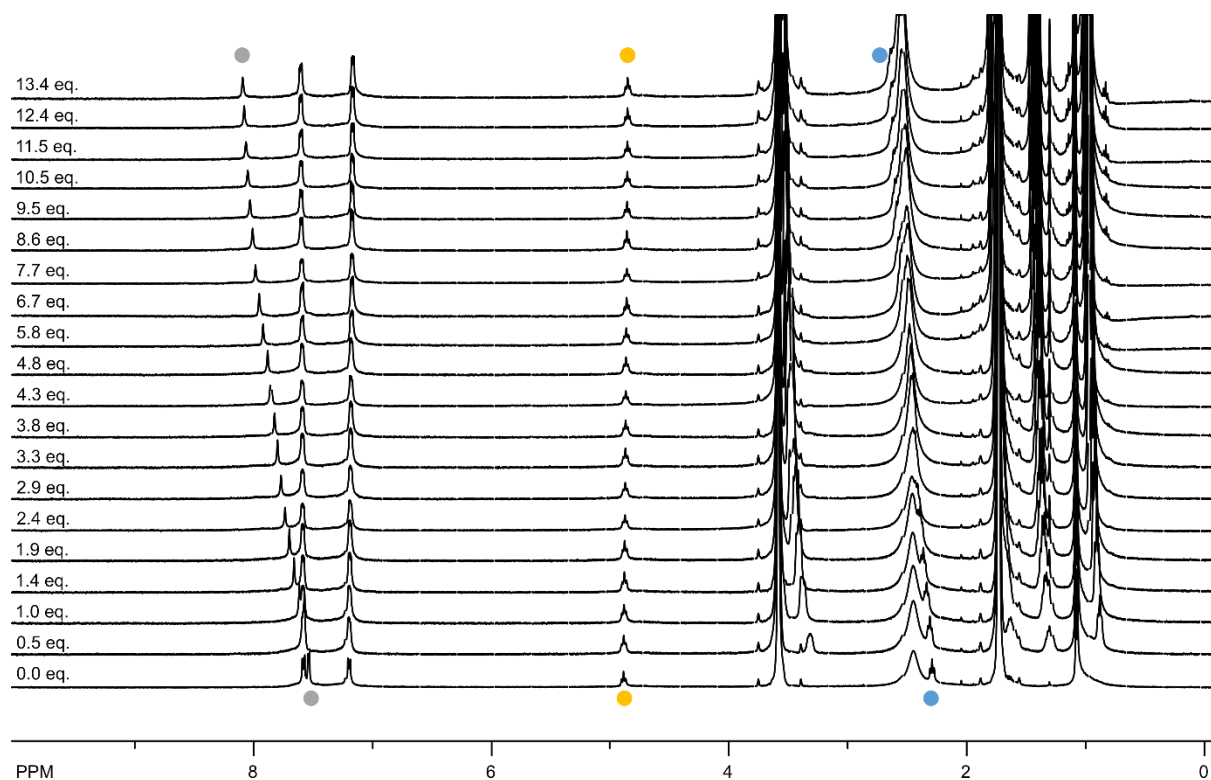
a)



K	error	SSR
$68 \text{ M}^{-1}$	0.9%	0.00185557

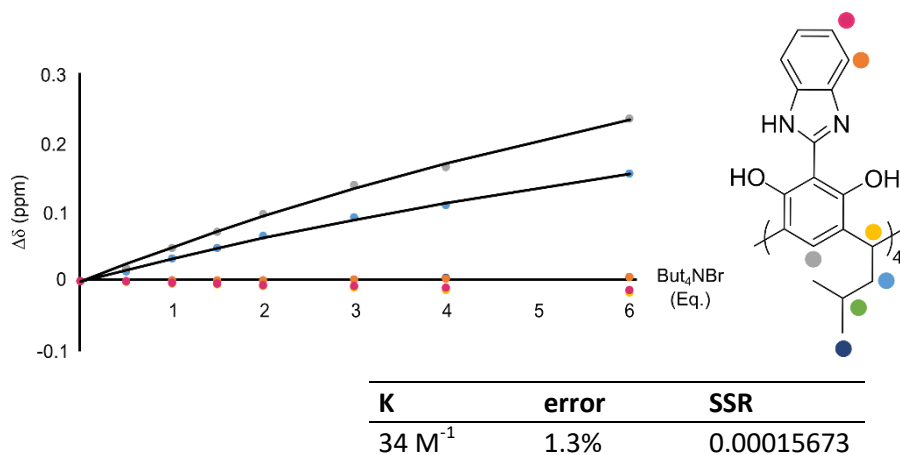
<http://app.supramolecular.org/bindfit/view/b8e4ef57-a2cd-4ddf-80e2-f33ed77a775a>

b)



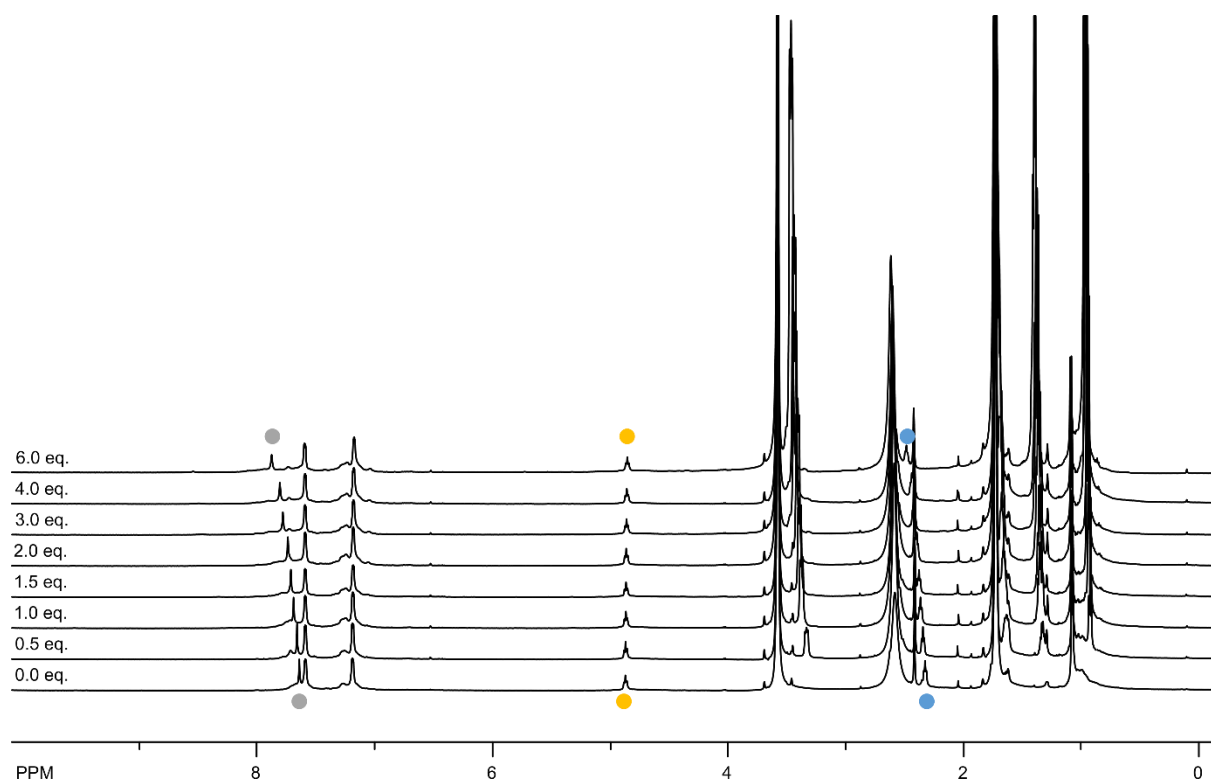
**Figure S14.**  $^1\text{H}$  NMR titration of **4** ( $C = 2 \text{ mM}$ ) with  $\text{But}_4\text{NBr}$  in  $[\text{D}_8]\text{THF}$ : a) experimental points and fitted curves (black lines, fitted using Bindfit); b)  $^1\text{H}$  NMR spectra (400 MHz, 303 K).

a)



<http://app.supramolecular.org/bindfit/view/f70b4b83-42ba-4059-b69e-0a8c92de0709>

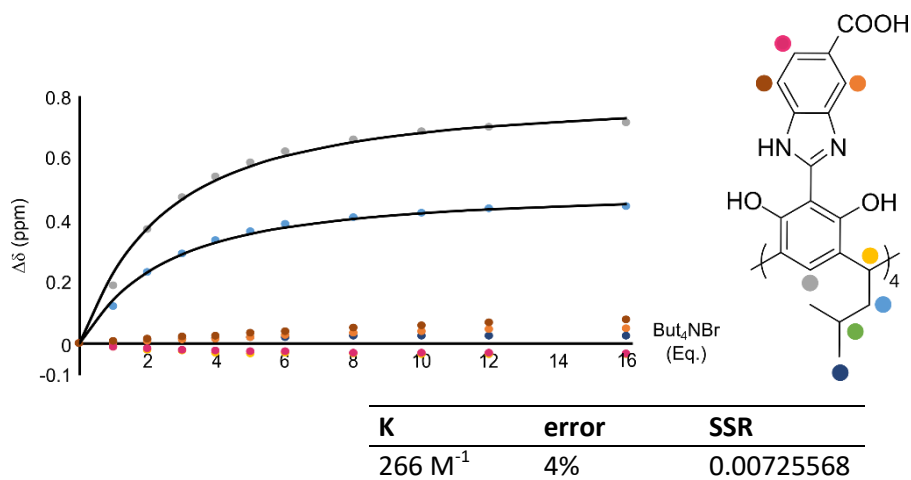
b)



**Figure S15.**  $^1\text{H}$  NMR titration of **4** ( $C = 2 \text{ mM}$ ) with  $\text{But}_4\text{NBr}$  in 98:2 ( $v:v$ )  $[\text{D}_8]\text{THF}:[\text{D}_6]\text{DMSO}$ : a) experimental points and fitted curves (black lines, fitted using Bindfit); b)  $^1\text{H}$  NMR spectra (600 MHz, 298 K).

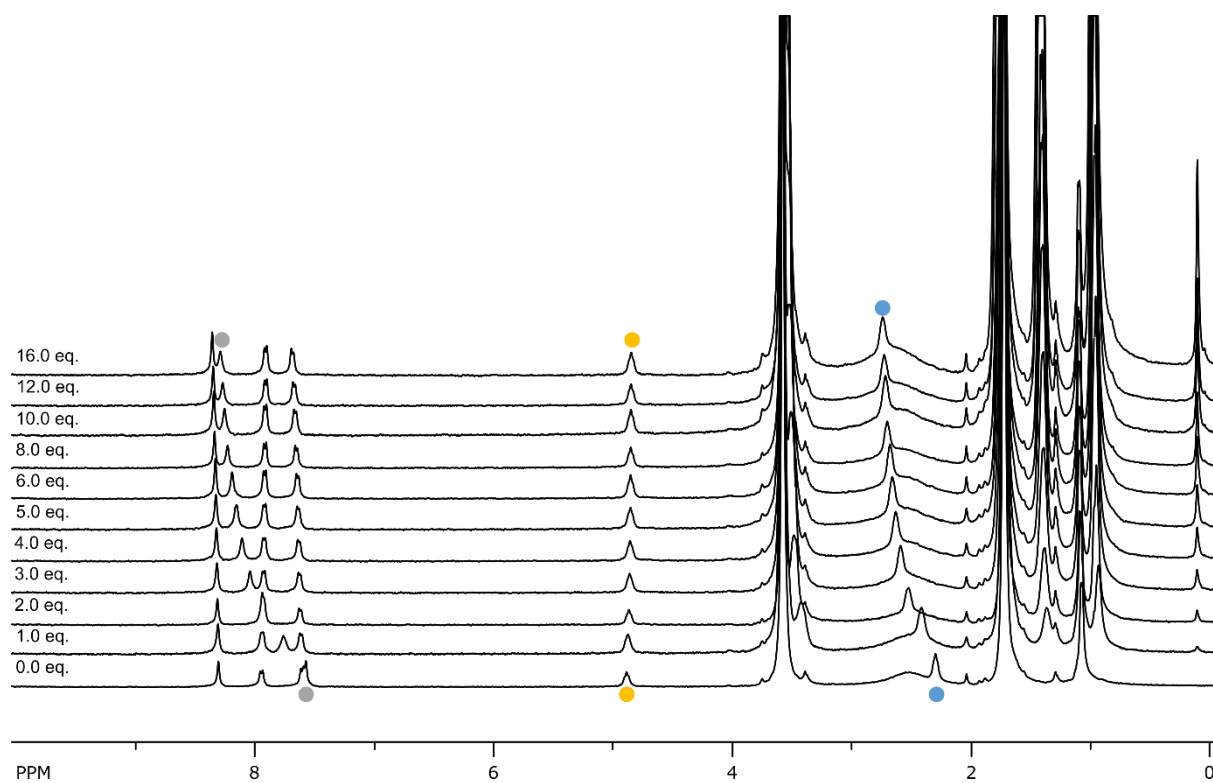
### 3.2 Titrations of 5 with But<sub>4</sub>NX in various solvents

a)



<http://app.supramolecular.org/bindfit/view/de374a4e-169b-4f76-86ad-dfc1d50c5edc>

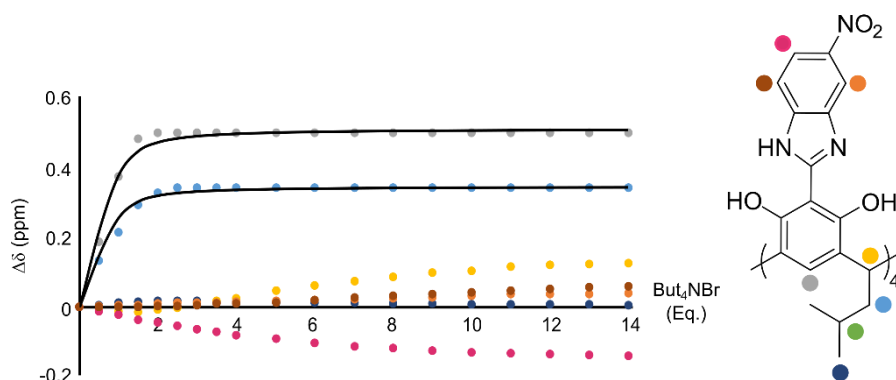
b)



**Figure S16.** <sup>1</sup>H NMR titration of 5 (C = 2 mM) with But<sub>4</sub>NBr in [D<sub>8</sub>]THF: a) experimental points and fitted curves (black lines, fitted using Bindfit); b) <sup>1</sup>H NMR spectra (400 MHz, 303 K).

### 3.3 Titrations of 6 with But<sub>4</sub>NX in various solvents

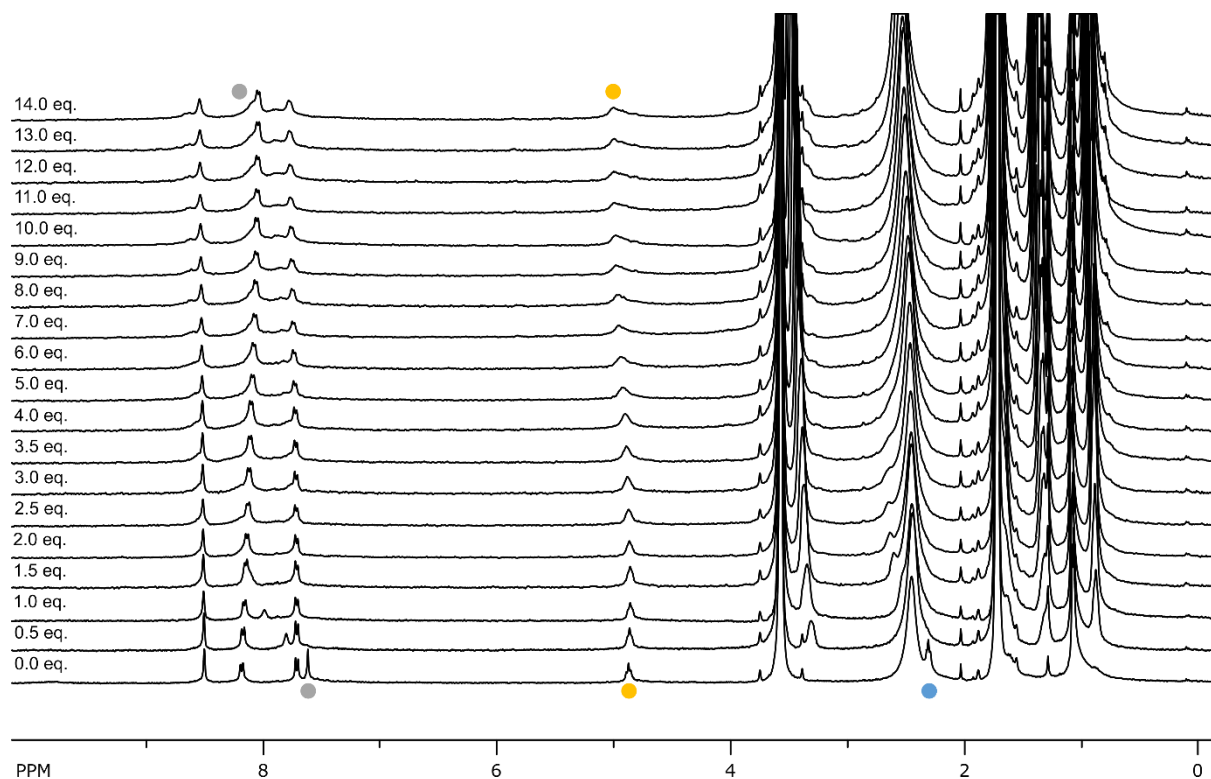
a)



K	error	SSR
6000 M <sup>-1</sup>	24%	0.00681759

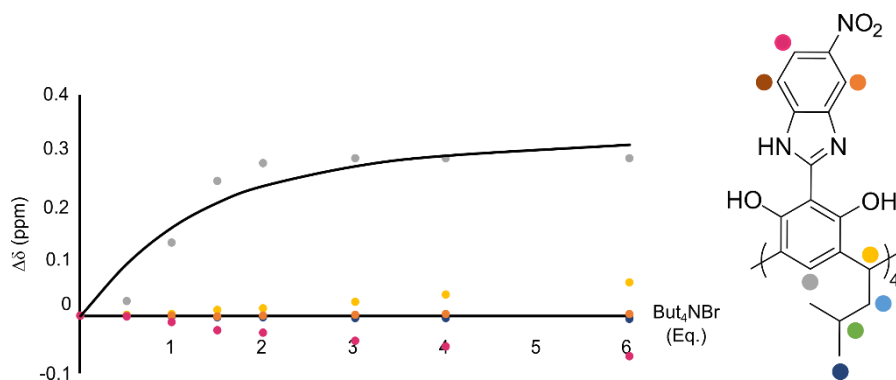
<http://app.supramolecular.org/bindfit/view/a2695f96-266a-4a14-82c7-e028c2c92365>

b)



**Figure S17.** <sup>1</sup>H NMR titration of **6** (C = 2 mM) with But<sub>4</sub>NBr in [D<sub>8</sub>]THF: a) experimental points and fitted curves (black lines, fitted using Bindfit); b) <sup>1</sup>H NMR spectra (400 MHz, 303 K).

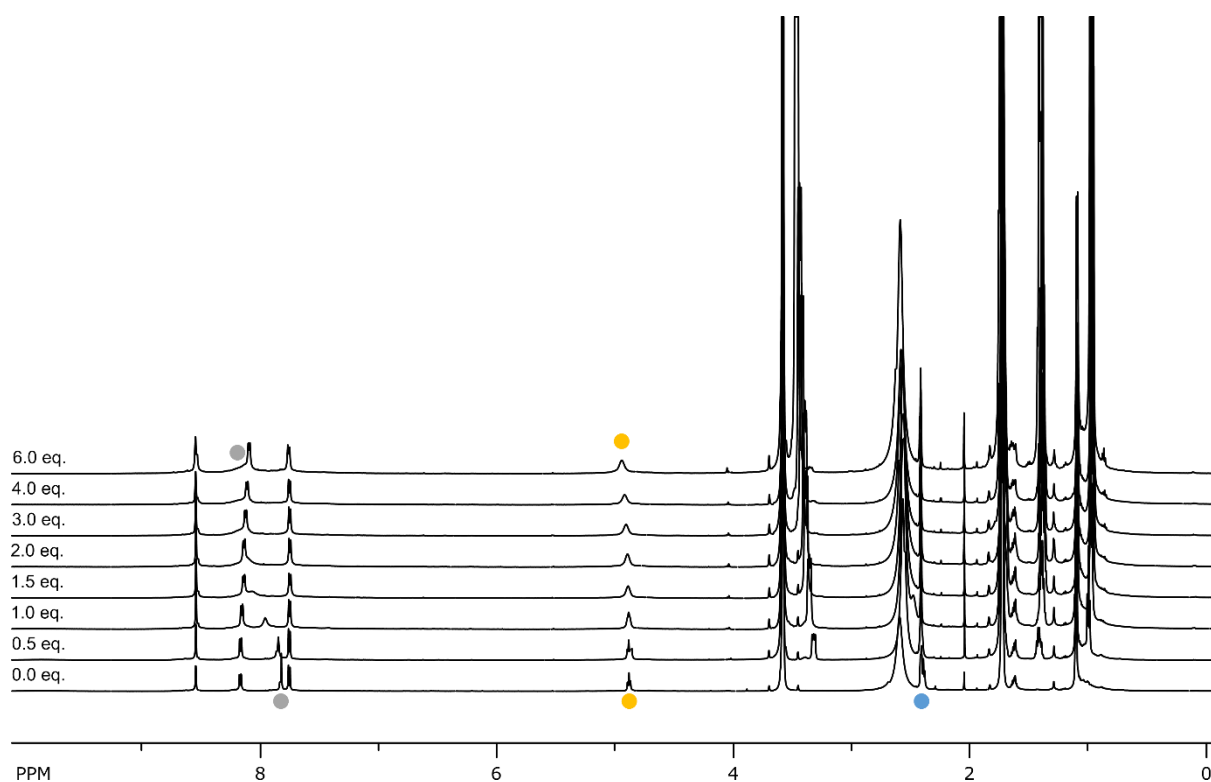
a)



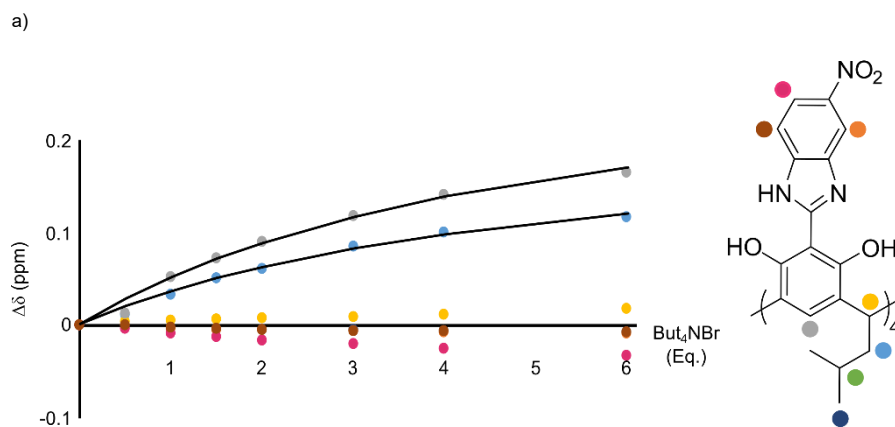
K	error	SSR
$780 \text{ M}^{-1}$	24%	0.01194784

<http://app.supramolecular.org/bindfit/view/65d1e613-7d5a-417c-9c61-7e684d9ea6ca>

b)

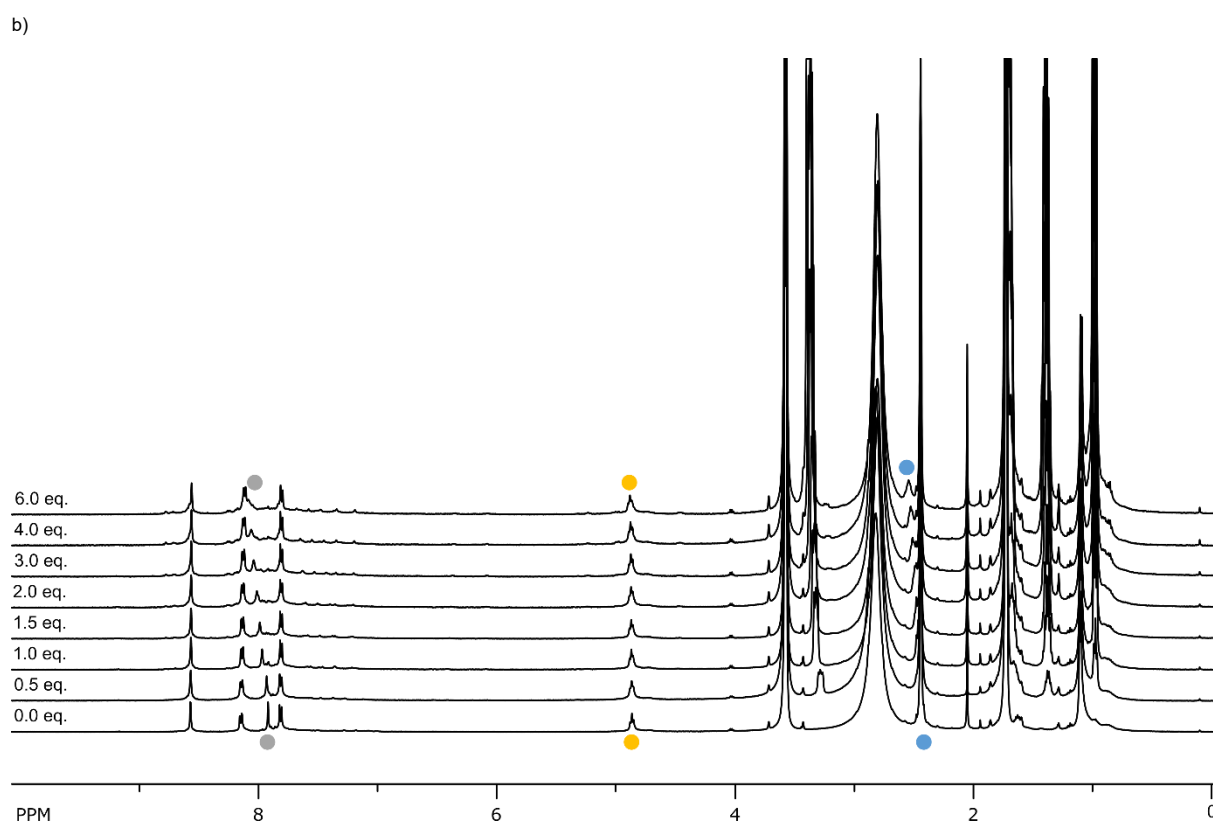


**Figure S18.**  $^1\text{H}$  NMR titration of **6** ( $C = 2 \text{ mM}$ ) with  $\text{But}_4\text{NBr}$  in 98:2 (v:v)  $[\text{D}_8]\text{THF}:[\text{D}_6]\text{DMSO}$ : a) experimental points and fitted curves (black lines, fitted using Bindfit); b)  $^1\text{H}$  NMR spectra (600 MHz, 298 K).



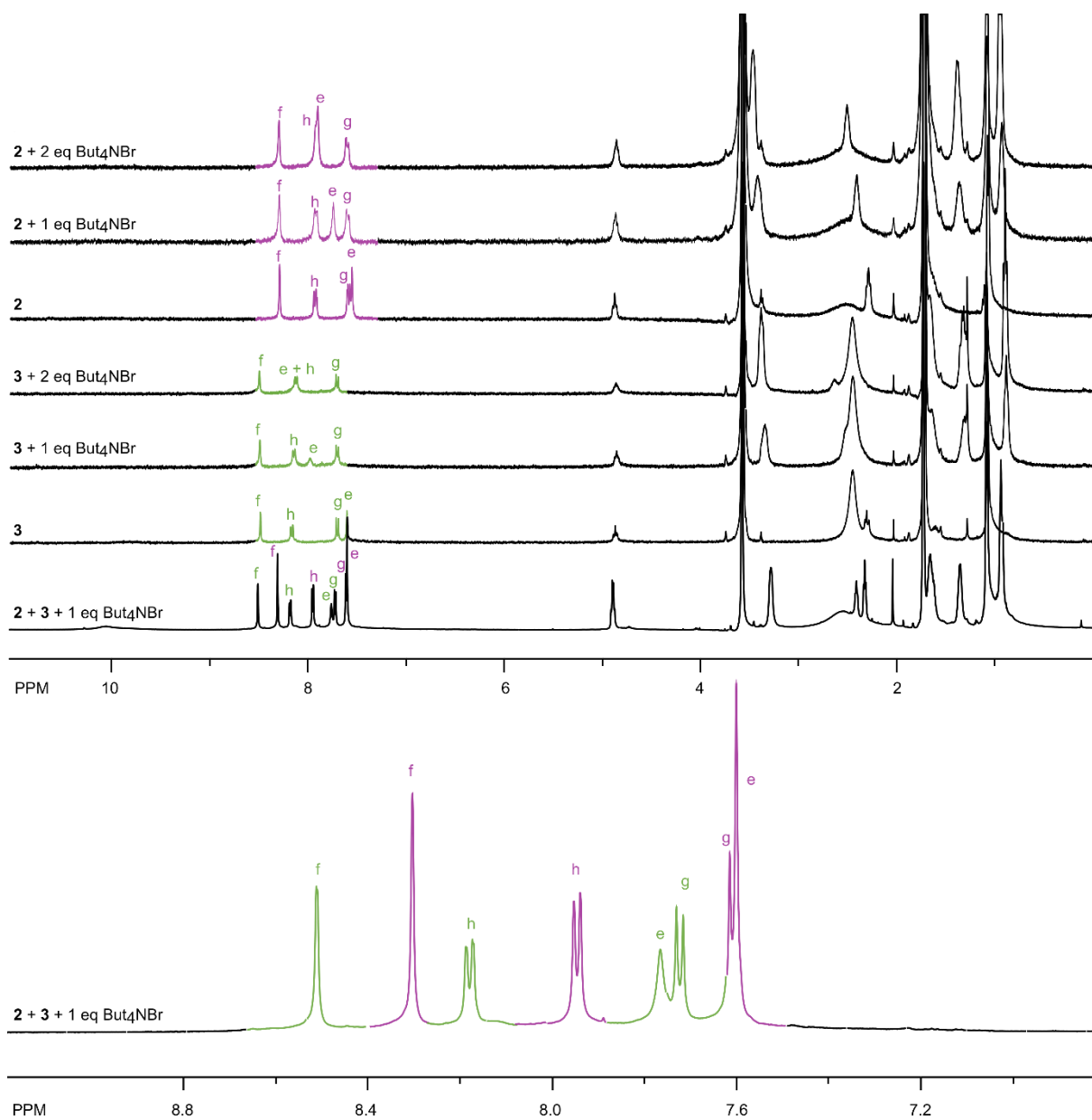
K	error	SSR
124 M <sup>-1</sup>	3%	0.0003778

<http://app.supramolecular.org/bindfit/view/24996170-1e72-432a-9805-9d7d8f2987c0>

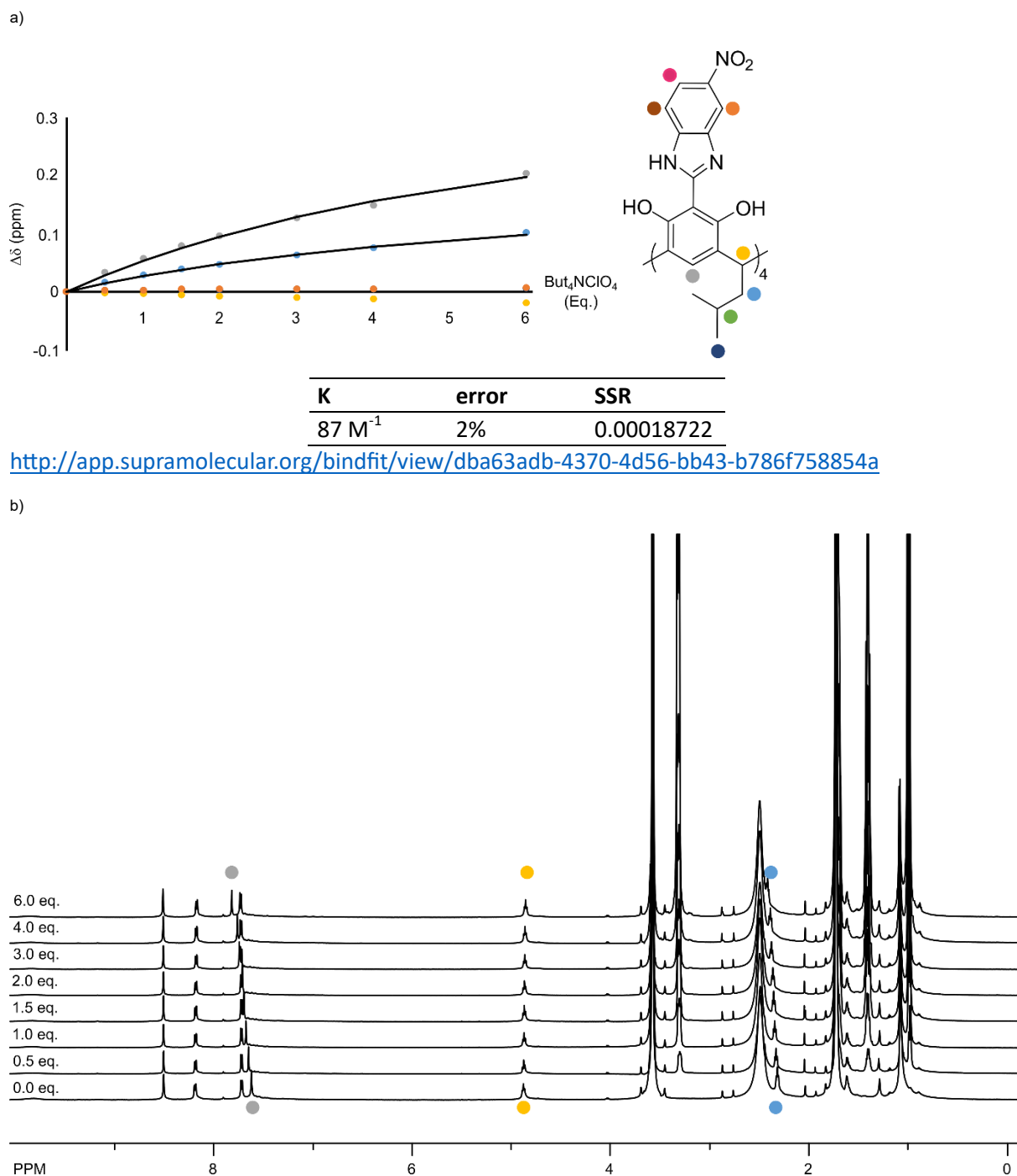


**Figure S19.** <sup>1</sup>H NMR titration of **6** (C = 2 mM) with But<sub>4</sub>NBr in 90:10 (v:v) [D<sub>8</sub>]THF:[D<sub>6</sub>]DMSO: a) experimental points and fitted curves (black lines, fitted using Bindfit); b) <sup>1</sup>H NMR spectra (500 MHz, 298 K).





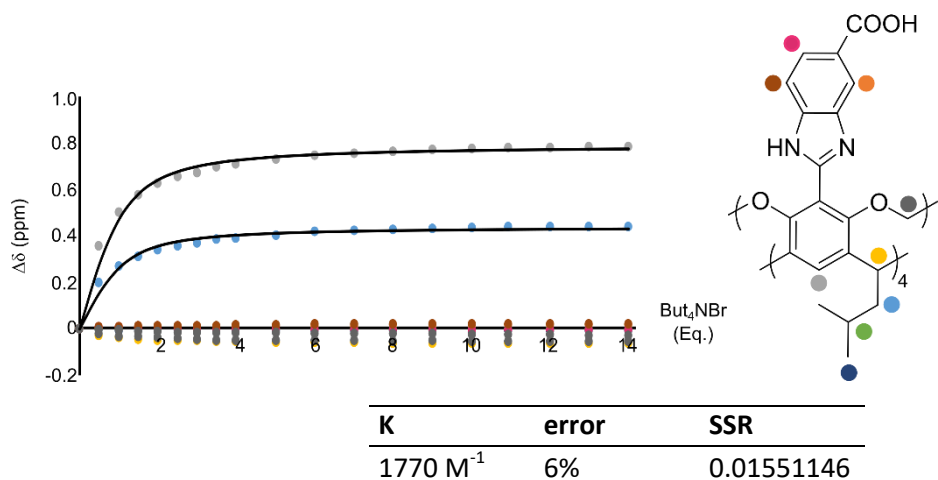
**Figure S20.**  $^1\text{H}$  NMR spectra of **5** and **6** (C = 2 mM each) with  $\text{But}_4\text{NBr}$ , ( $[\text{D}_8]\text{THF}$ , 600 MHz, 298 K).



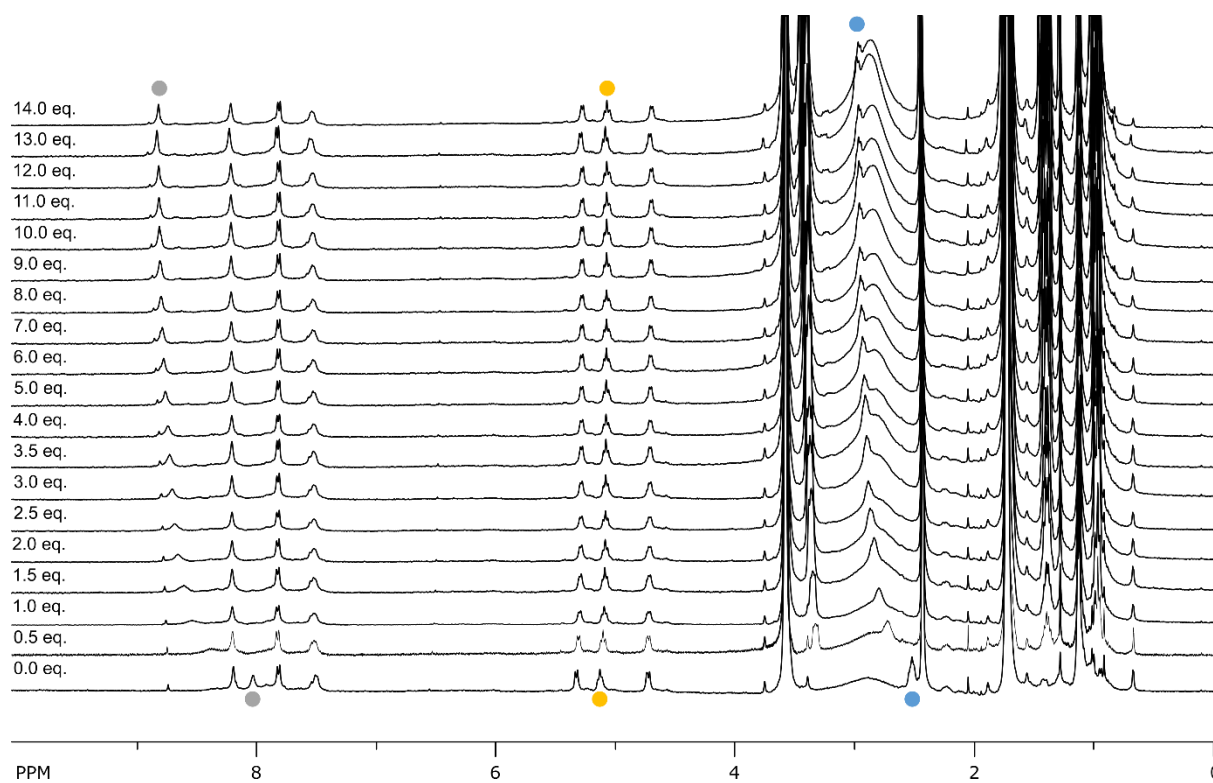
**Figure S21.**  $^1\text{H}$  NMR titration of **6** ( $C = 2 \text{ mM}$ ) with  $\text{But}_4\text{NClO}_4$  in  $[\text{D}_8]\text{THF}$ : a) experimental points and fitted curves (black lines, fitted using Bindfit); b)  $^1\text{H}$  NMR spectra (600 MHz, 298 K).

### 3.4 Titrations of **8** with But<sub>4</sub>NX in various solvents

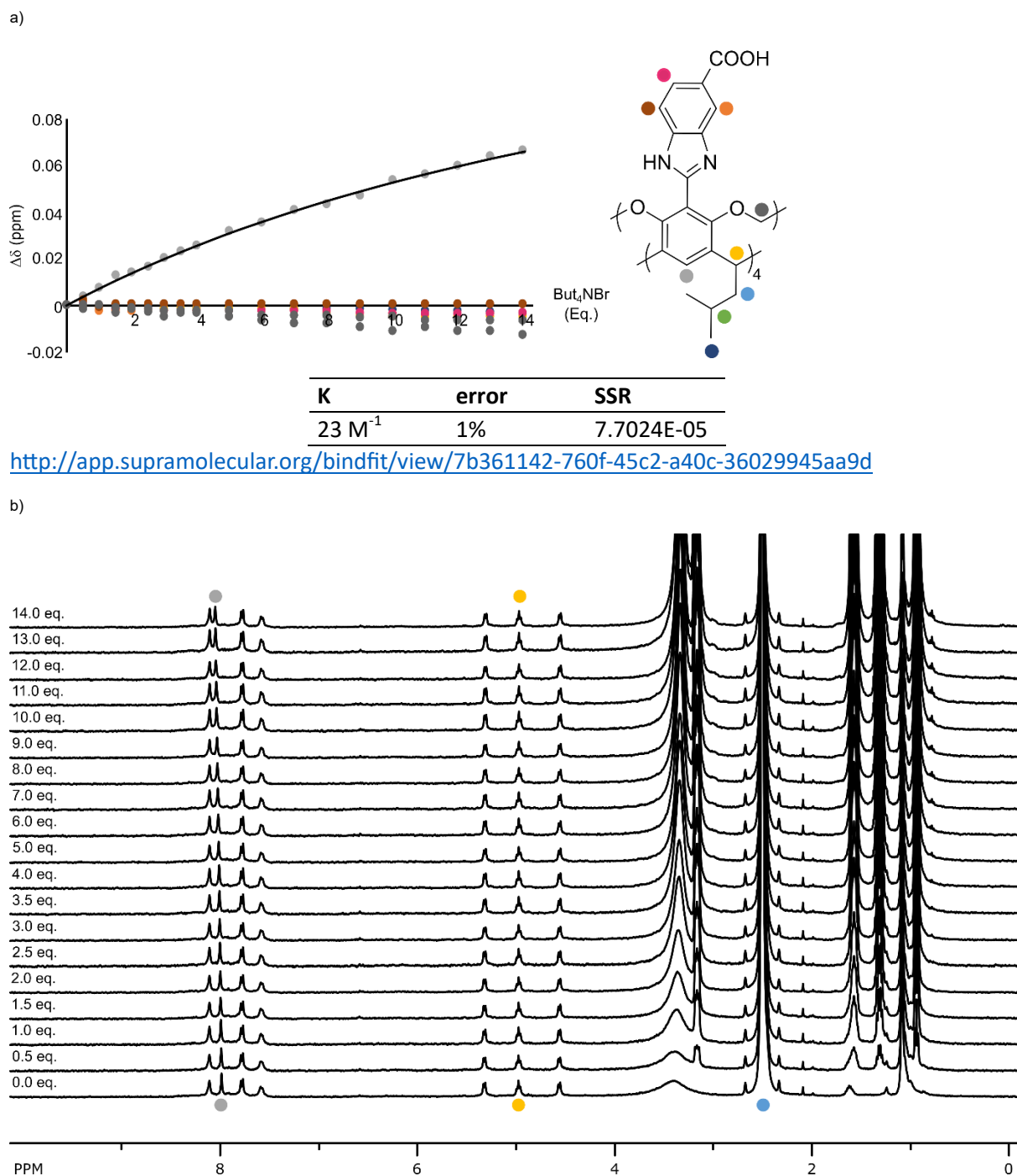
a)



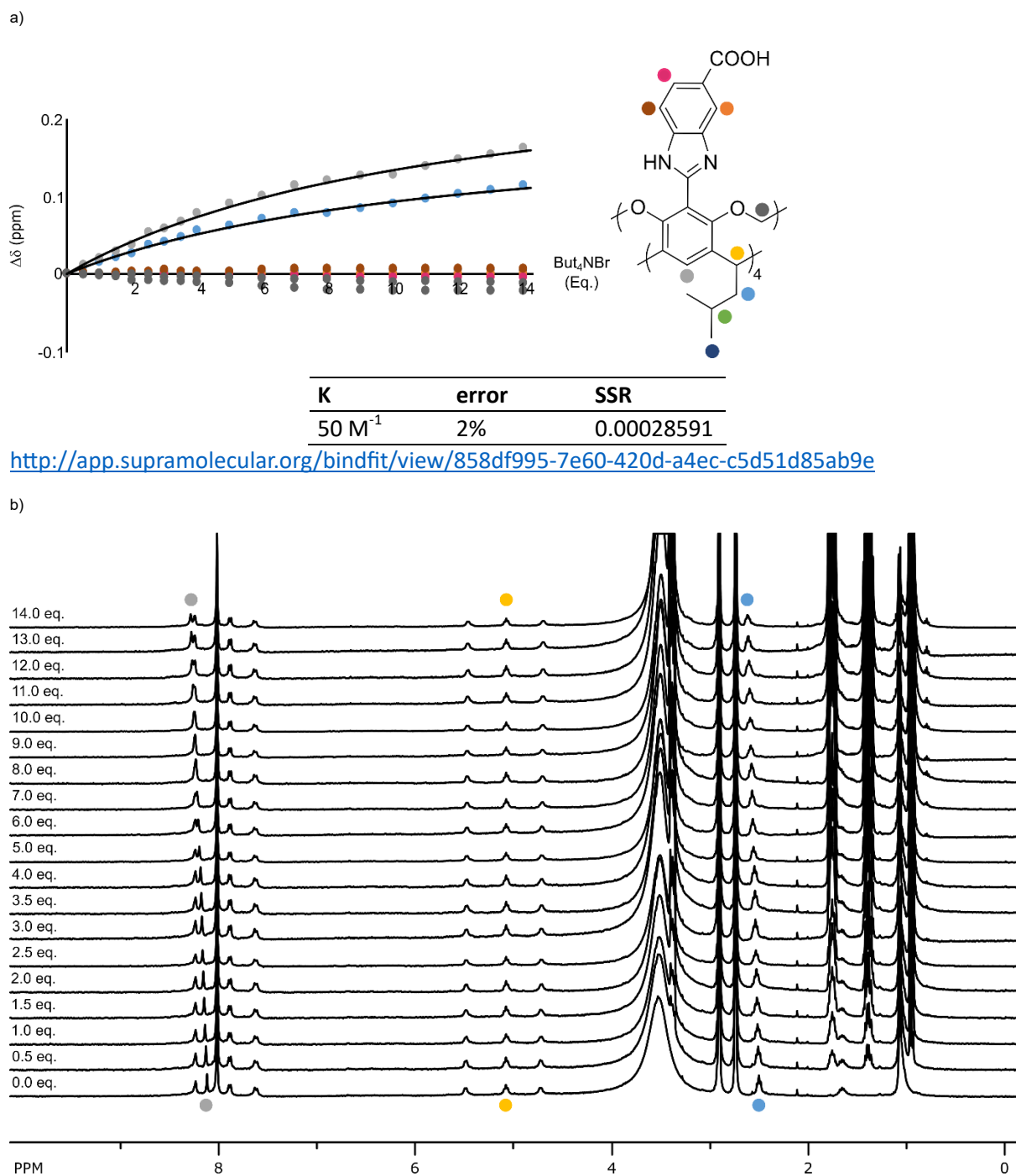
b)



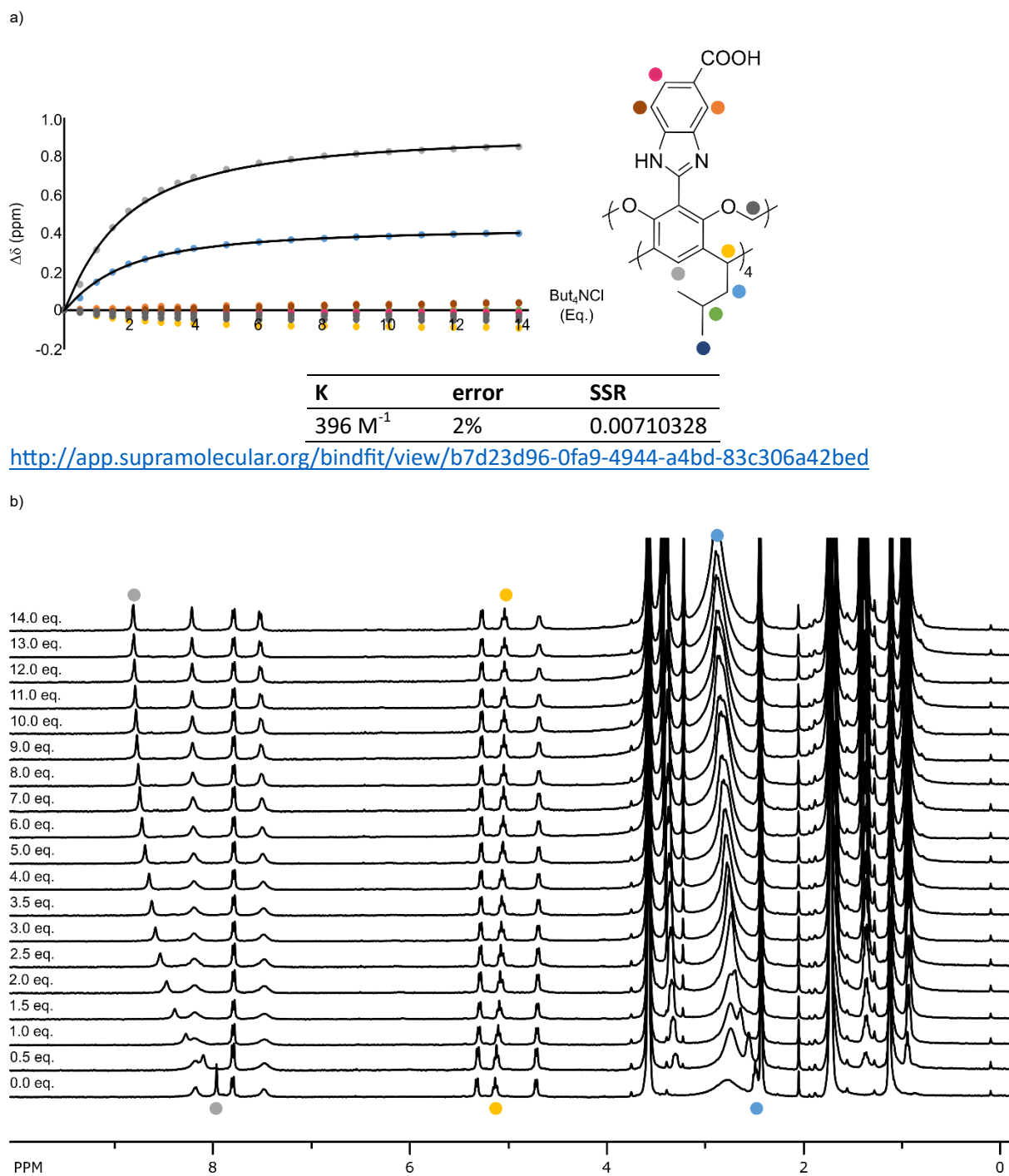
**Figure S22.** <sup>1</sup>H NMR titration of **8** (C = 2 mM) with But<sub>4</sub>NBr in 90:10 (v:v) [D<sub>8</sub>]THF:[D<sub>6</sub>]DMSO: a) experimental points and fitted curves (black lines, fitted using Bindfit); b) <sup>1</sup>H NMR spectra (400 MHz).



**Figure S23.** <sup>1</sup>H NMR titration of **8** (C = 2 mM) with But<sub>4</sub>NBr in [D<sub>6</sub>]DMSO: a) experimental points and fitted curves (black lines, fitted using Bindfit); b) <sup>1</sup>H NMR spectra (400 MHz, 303 K).



**Figure S24.** <sup>1</sup>H NMR titration of **8** (C = 2 mM) with But<sub>4</sub>NBr in [D<sub>7</sub>]DMF: a) experimental points and fitted curves (black lines, fitted using Bindfit); b) <sup>1</sup>H NMR spectra (400 MHz, 303 K).

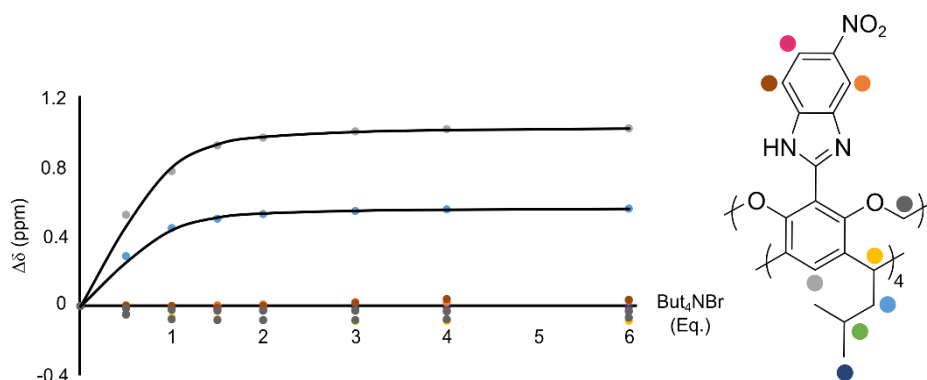


**Figure S25.** <sup>1</sup>H NMR titration of **8** (C = 2 mM) with But<sub>4</sub>NCl in 90:10 (v:v) [D<sub>8</sub>]THF:[D<sub>6</sub>]DMSO: a) experimental points and fitted curves (black lines, fitted using Bindfit); b) <sup>1</sup>H NMR spectra (400 MHz, 303 K).



### 3.5 Titrations of 9 with But<sub>4</sub>NX in various solvents

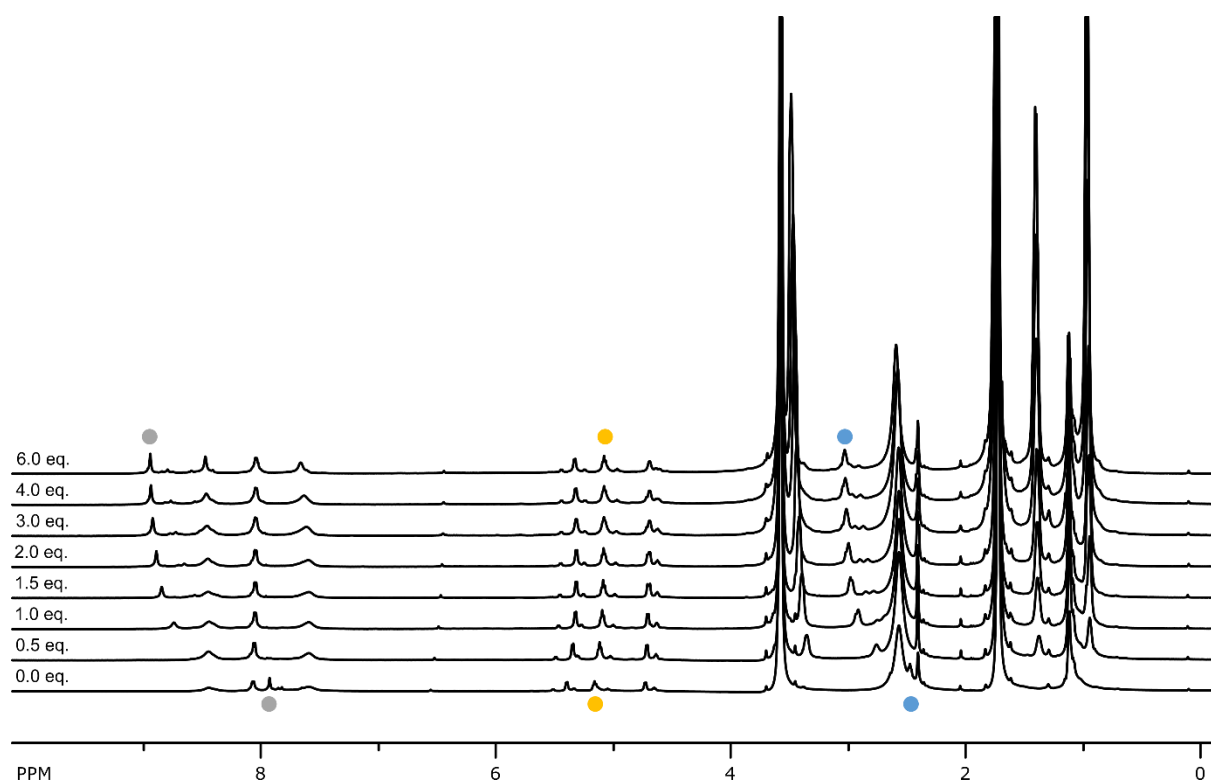
a)



K	error	SSR
7000 M <sup>-1</sup>	14%	0,008858681

<http://app.supramolecular.org/bindfit/view/ca42f4f7-799c-43ec-8be3-1ce1fb948e60>

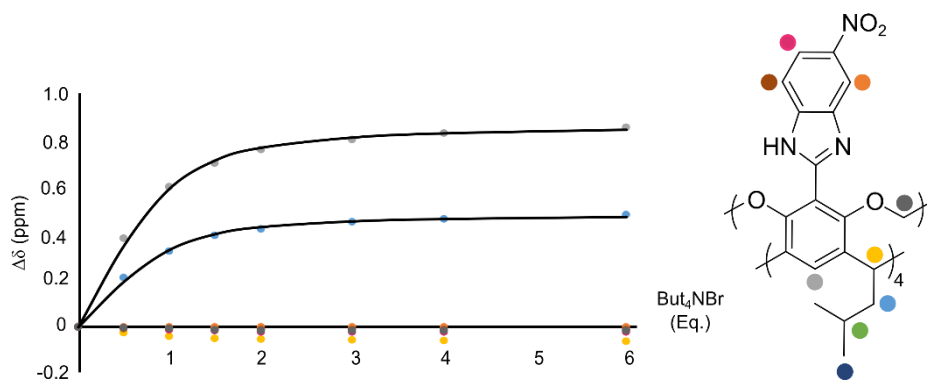
b)



**Figure S27.** <sup>1</sup>H NMR titration of **9** (C = 2 mM) with But<sub>4</sub>NBr in 98:2 (v:v) [D<sub>8</sub>]THF:[D<sub>6</sub>]DMSO: a) experimental points and fitted curves (black lines, fitted using Bindfit); b) <sup>1</sup>H NMR spectra (600 MHz, 298 K).



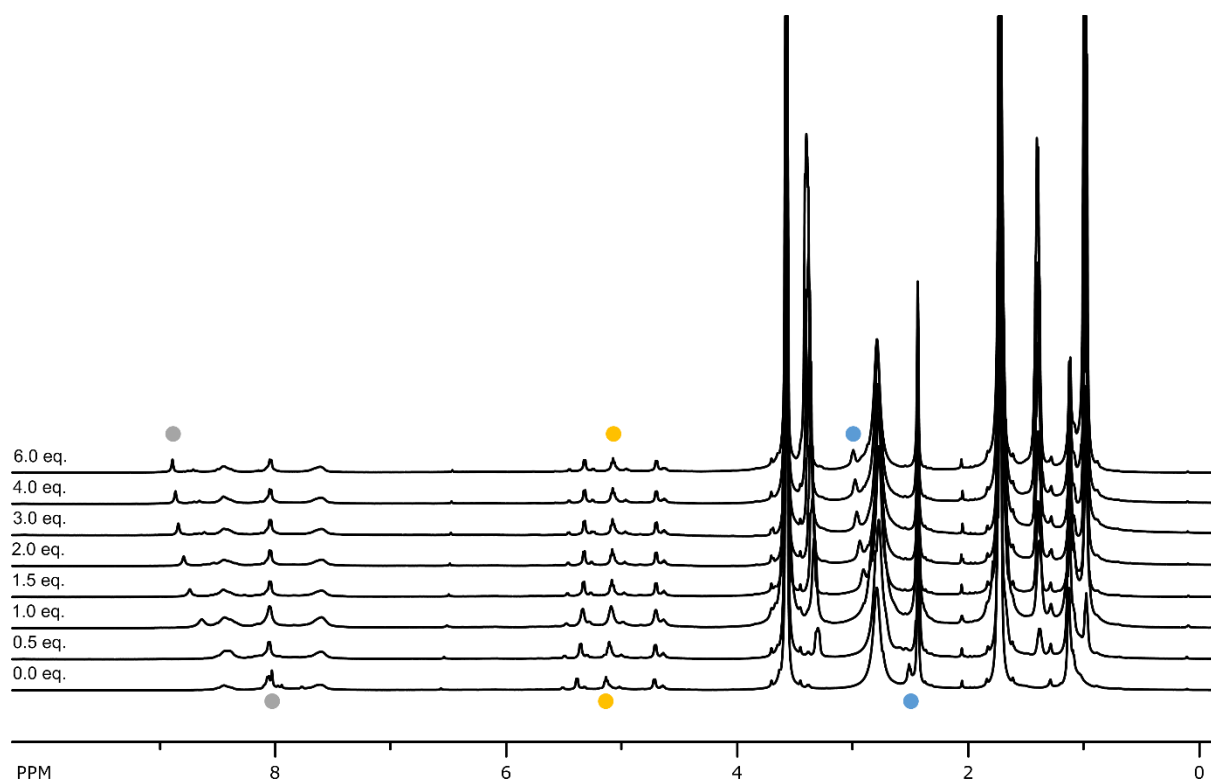
a)



K	error	SSR
3363 M <sup>-1</sup>	6%	0.00198003

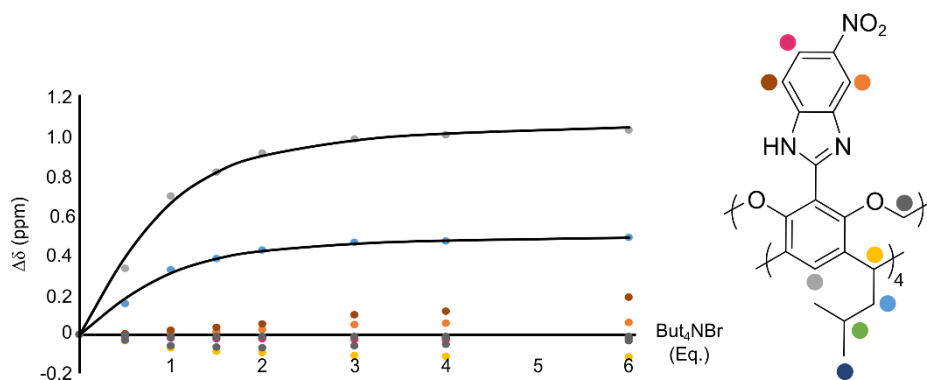
<http://app.supramolecular.org/bindfit/view/6fb98fab-8055-419a-b2fa-fbe92e79550d>

b)



**Figure S28.** <sup>1</sup>H NMR titration of **9** (C = 2 mM) with But<sub>4</sub>NBr in 90:10 (v:v) [D<sub>8</sub>]THF:[D<sub>6</sub>]DMSO: a) experimental points and fitted curves (black lines, fitted using Bindfit); b) <sup>1</sup>H NMR spectra (600 MHz, 298 K).

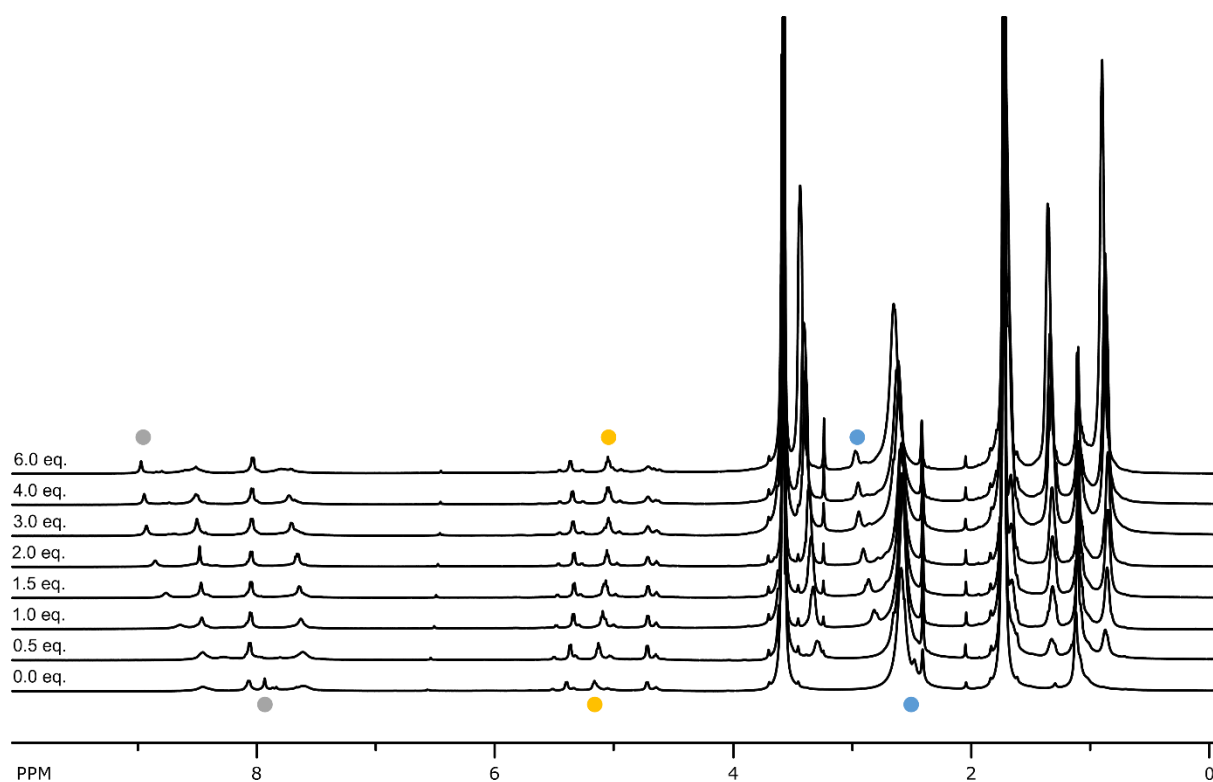
a)



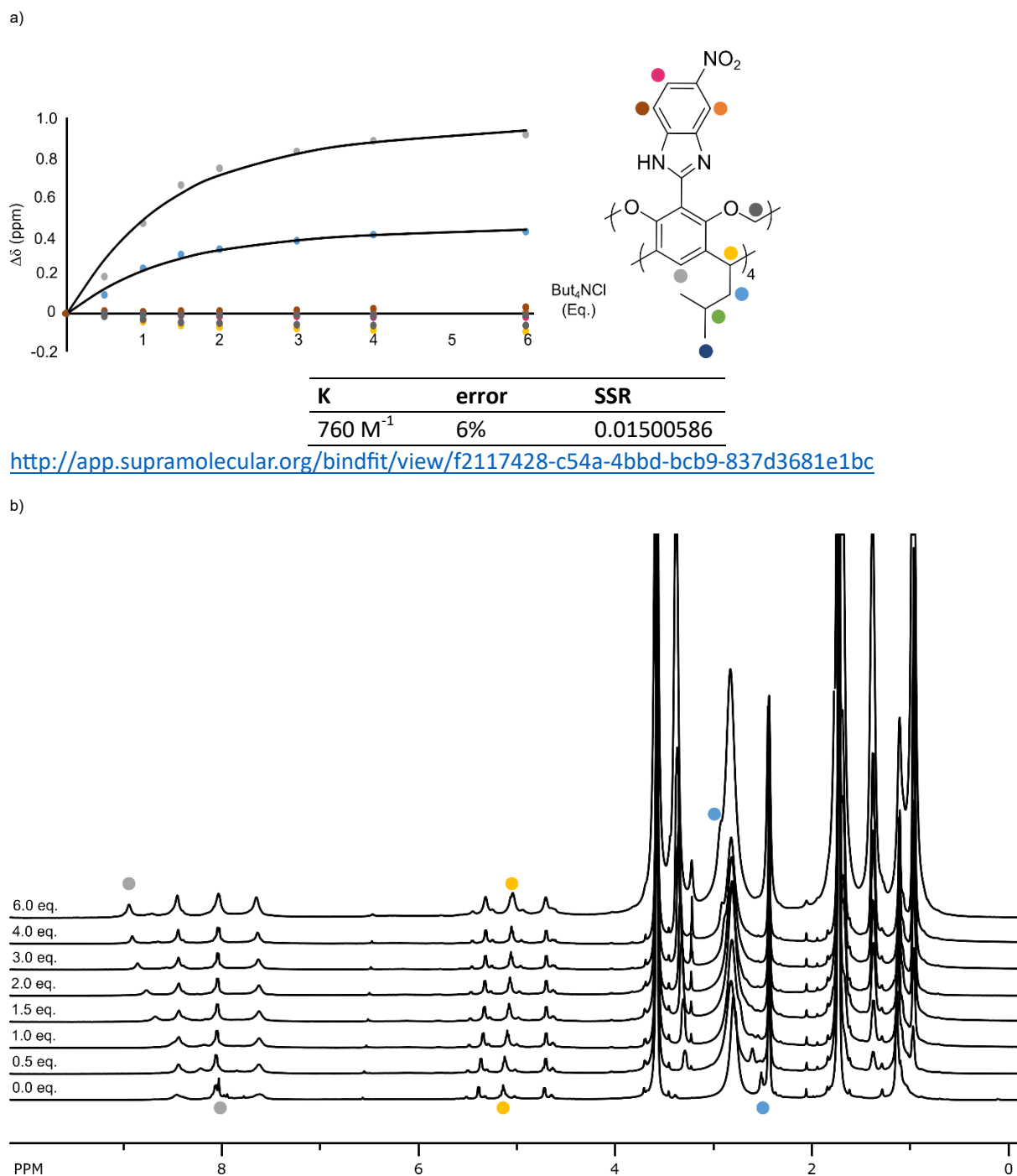
K	error	SSR
1900 M <sup>-1</sup>	11%	0.02435714

<http://app.supramolecular.org/bindfit/view/2ae6d39e-c25f-4035-9c20-e6d0cd60a2bd>

b)

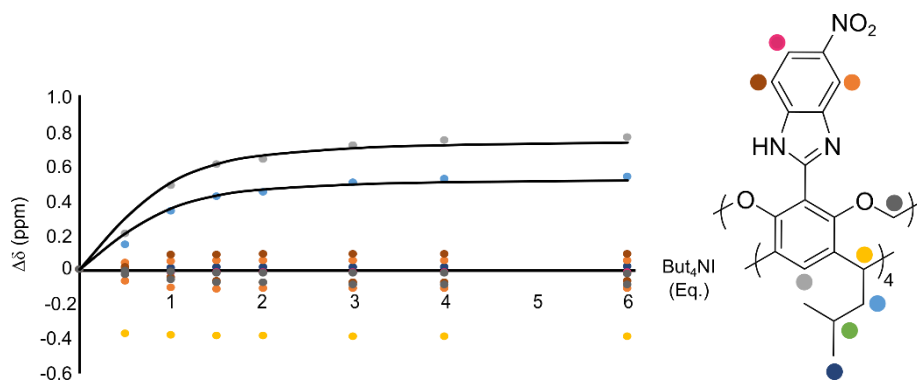


**Figure S29.** <sup>1</sup>H NMR titration of **9** (C = 2 mM) with But<sub>4</sub>NCl in 98:2 (v:v) [D<sub>8</sub>]THF:[D<sub>6</sub>]DMSO: a) experimental points and fitted curves (black lines, fitted using Bindfit); b) <sup>1</sup>H NMR spectra (600 MHz, 298 K).



**Figure S30.** <sup>1</sup>H NMR titration of **9** (C = 2 mM) with But<sub>4</sub>NCl in 90:10 (v:v) [D<sub>8</sub>]THF:[D<sub>6</sub>]DMSO: a) experimental points and fitted curves (black lines, fitted using Bindfit); b) <sup>1</sup>H NMR spectra (600 MHz, 298 K).

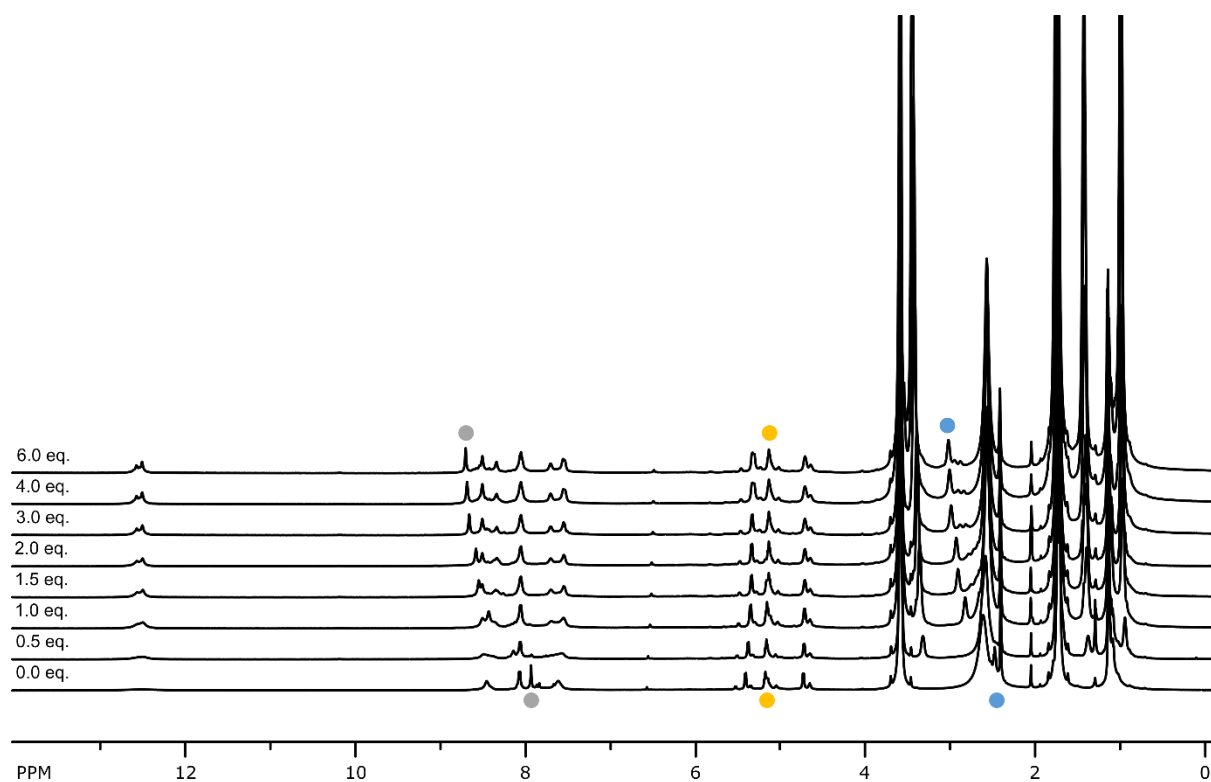
a)



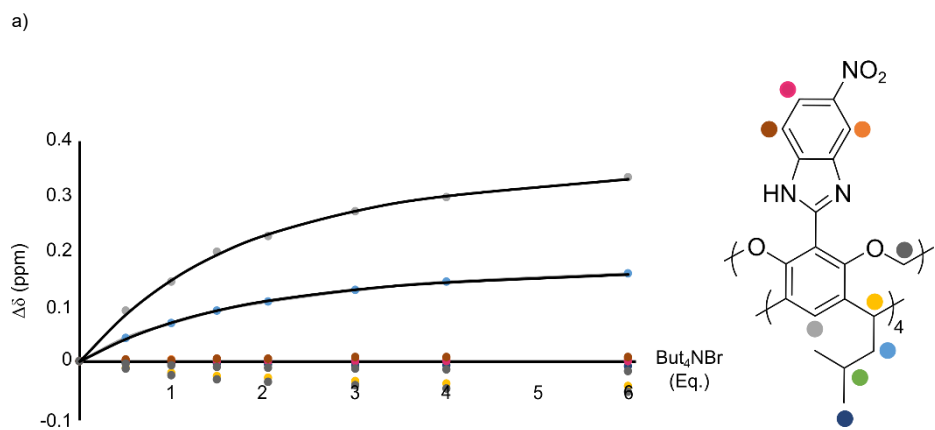
K	error	SSR
2900 M <sup>-1</sup>	23%	0.0693411

<http://app.supramolecular.org/bindfit/view/49a3e702-8e39-4a16-9960-a791c9ff961e>

b)

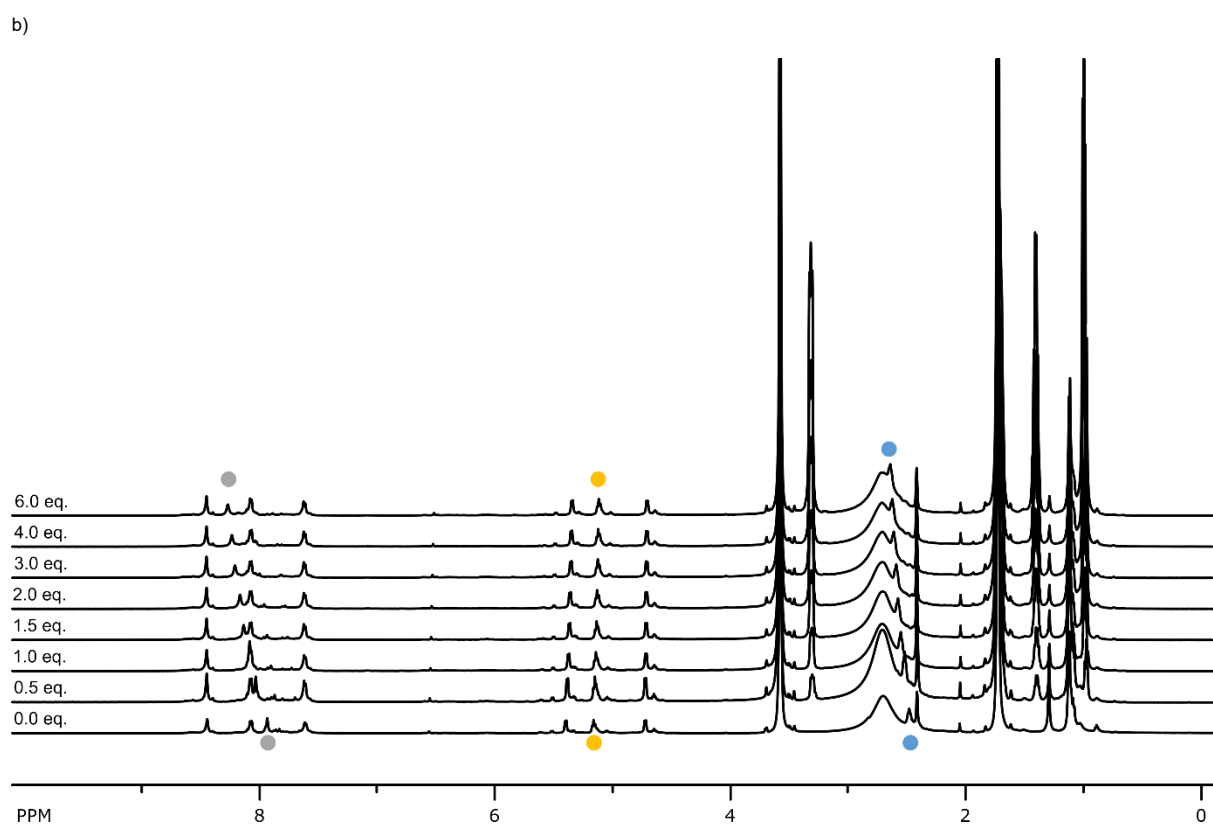


**Figure S31.** <sup>1</sup>H NMR titration of **9** (C = 2 mM) with But<sub>4</sub>NI in 98:2 (v:v) [D<sub>8</sub>]THF:[D<sub>6</sub>]DMSO: a) experimental points and fitted curves (black lines, fitted using Bindfit); b) <sup>1</sup>H NMR spectra (600 MHz, 298 K).



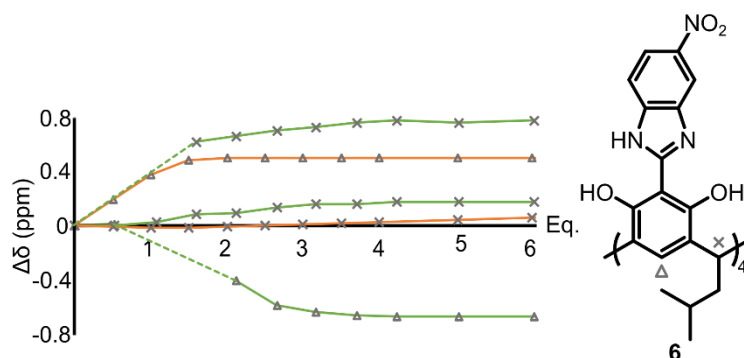
K	error	SSR
450 M <sup>-1</sup>	2%	0.00016448

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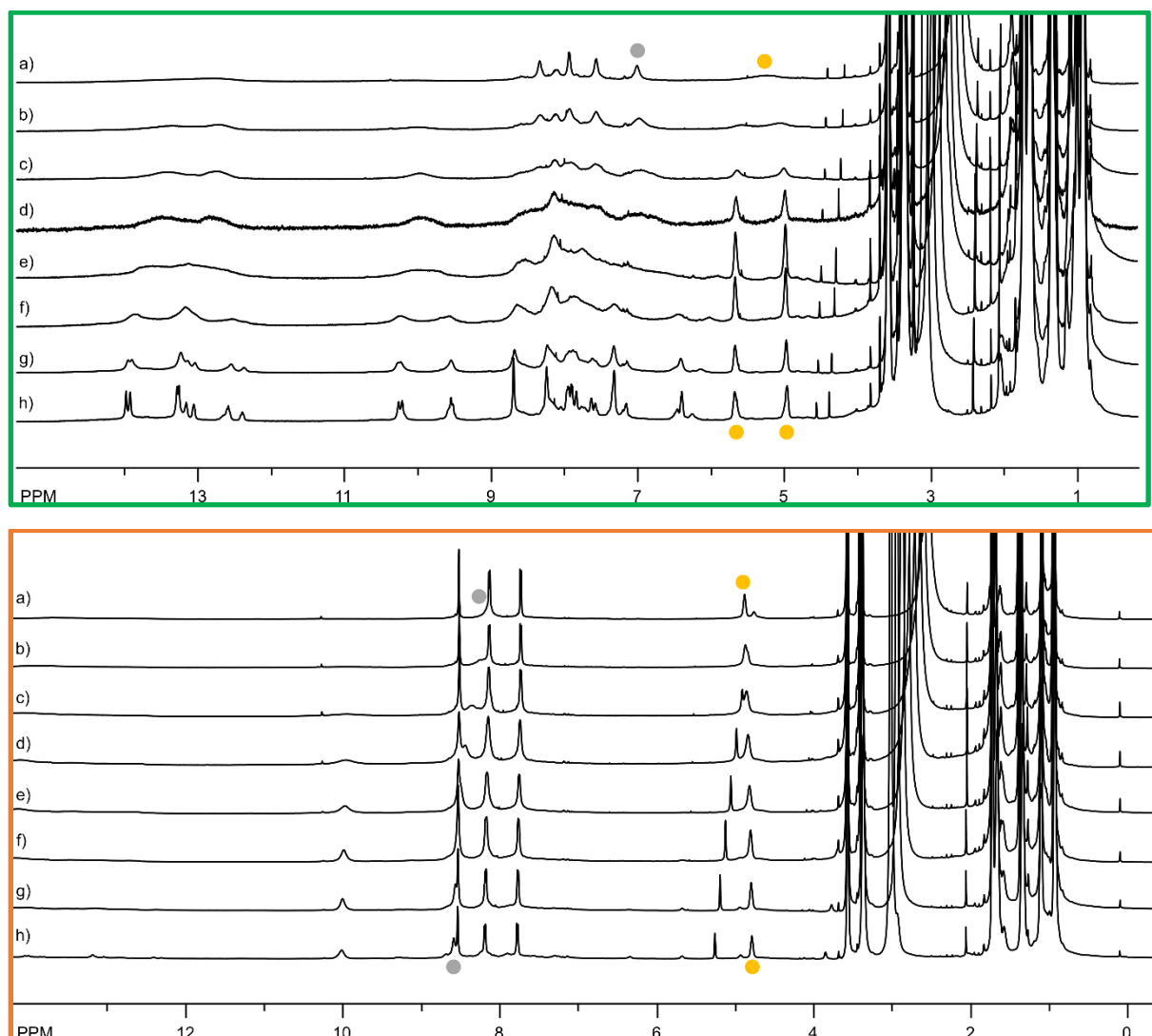


**Figure S32.** <sup>1</sup>H NMR titration of **9** (C = 2 mM) with But<sub>4</sub>NClO<sub>4</sub> in 98:2 (v:v) [D<sub>8</sub>]THF:[D<sub>6</sub>]DMSO: a) experimental points and fitted curves (black lines, fitted using Bindfit); b) <sup>1</sup>H NMR spectra (600 MHz, 298 K).

#### 4. Comparison of Cl<sup>-</sup> and Br<sup>-</sup> complexation by receptor **6** and VT NMR spectra



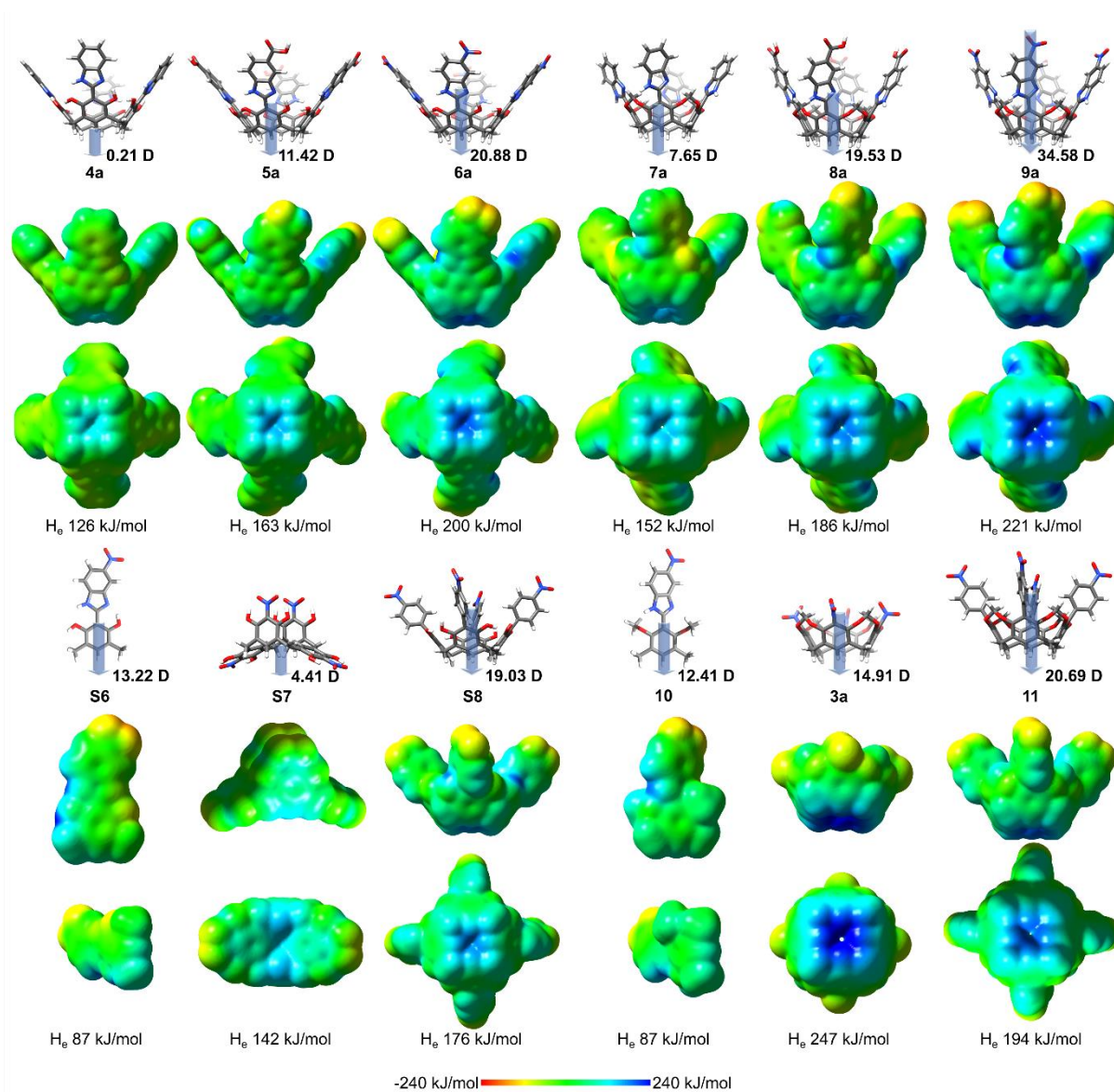
**Figure S33.** Changes in chemical shifts observed during titration of **6** (C = 2 mM) with But<sub>4</sub>NCl (—x—, dashed lines in the area where signals were not visible) or But<sub>4</sub>NBr (—△—)



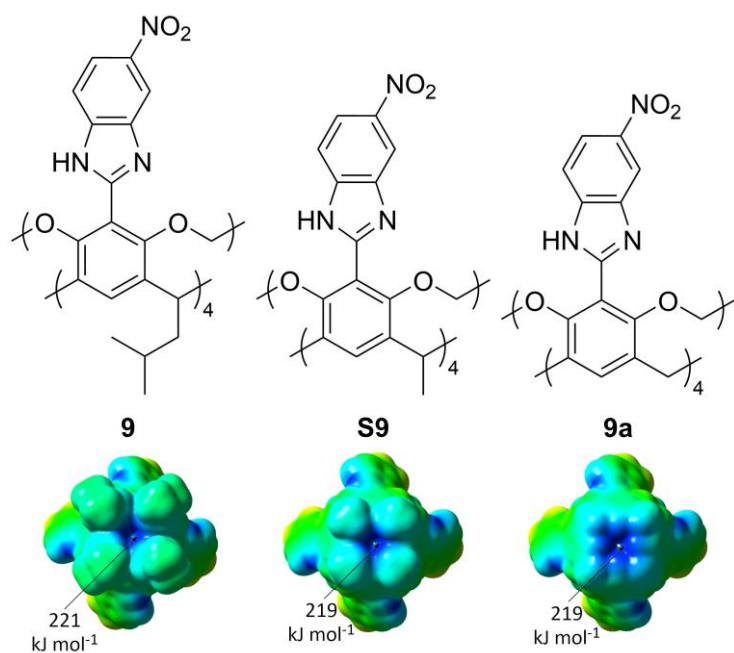
**Figure S34.** VT <sup>1</sup>H NMR spectra of **6** (C = 2 mM) with 4 eq. But<sub>4</sub>NCl (4 eq., green panel) or 4 eq. But<sub>4</sub>NBr (4 eq., orange panel) at: a) 313 K, b) 303 K, c) 293 K, d) 283 K, e) 273 K, f) 263 K, g) 253 K, h) 243 K, i) 233 K (all in [D<sub>8</sub>]THF, 600 MHz).

## 5. Theoretical calculations

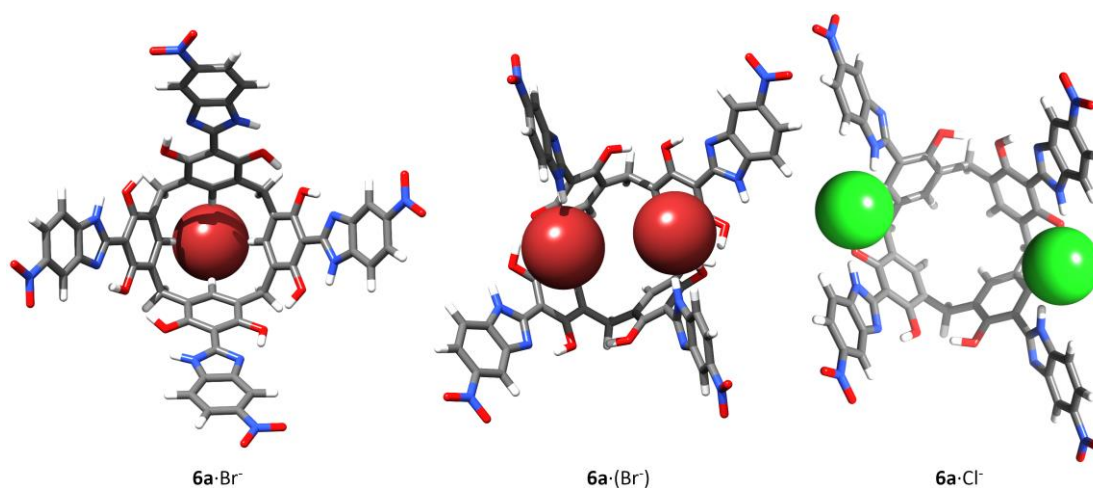
All calculations for cavitands and monomers forms were performed within the density functional theory (DFT) approach using Gaussian 16 program suite.<sup>5</sup> Geometry was optimized with the B3LYP functional, employing the 6-31+G(D,P) basis set. Solvent effects (THF) were considered within the SMD model. Atomic coordinates for optimized structures are listed below.



**Figure S35.** Theoretical calculation of geometry and electrostatic surface potentials (ESP). Geometry optimization by DFT B3LYP 6-31+G(D,P) in THF (SMD model); ESPs mapped onto electron density isosurfaces ( $0.0004 \text{ e au}^{-3}$ ).



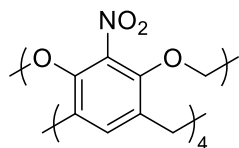
**Figure S36.** Theoretical calculation of geometry and electrostatic surface potentials (ESP). Geometry optimization by DFT B3LYP 6-31+G(D,P) in THF (SMD model); ESPs mapped onto electron density isosurfaces (0.0004 e au<sup>-3</sup>).



**Figure S37.** Theoretical calculation of geometry of complexes. Geometry optimization by DFT B3LYP 6-31+G(D,P) in THF (SMD model).



3a



Energy = -2653.714 Hartree

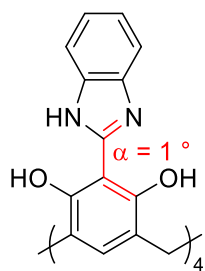
Number of imaginary frequencies 0

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O	-2.38639600	4.06466700	-0.28144500
O	2.38812300	4.07653200	-0.28047700
O	-4.07653200	2.38812300	-0.28047700
O	-4.06466700	-2.38639600	-0.28144500
C	3.09551400	3.10136900	-1.04517000
H	2.39666600	2.40743700	-1.51997900
H	3.66643900	3.66880300	-1.77846400
C	3.10136900	-3.09551400	-1.04517000
H	3.66880300	-3.66643900	-1.77846400
H	2.40743700	-2.39666600	-1.51997900
C	-3.10136900	3.09551400	-1.04517000
H	-2.40743700	2.39666600	-1.51997900
H	-3.66880300	3.66643900	-1.77846400
C	-3.09551400	-3.10136900	-1.04517000
H	-2.39666600	-2.40743700	-1.51997900
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N	4.79679900	0.01143200	-1.48772800

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H	3.30250700	-3.30774400	2.05105500
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C	2.99090500	1.22986100	1.56676700
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C	-3.69098900	1.22613100	0.34917900
O	4.19126000	0.32126000	-2.51460900
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H	0.00289800	2.15322100	3.10455000
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C	-2.99090500	-1.22986100	1.56676700
C	-1.22986100	2.99090500	1.56676700
C	2.68008600	-0.00147600	2.15398800
H	2.15322100	-0.00289800	3.10455000
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C	-0.00027500	4.03459300	-0.22811100
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O -4.19126000 -0.32126000 -2.51460900

4a



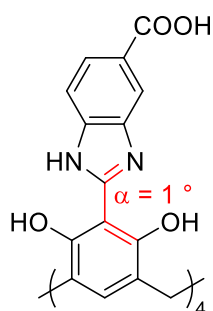
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Number of imaginary frequencies 0

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C	-7.38465800	-0.46649900	2.61629100	N	5.48238400	-1.97029500	0.84712300
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C	0.28211100	7.98750600	3.63798500	H	3.69445000	3.05468700	-1.06549300
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5a



Energy = -3952.6997 Hartree

Number of imaginary frequencies 0

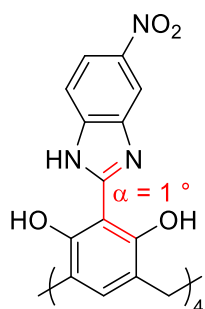
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C	3.12922700	1.73540700	-4.02785900
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C	3.39146800	-2.23371500	-2.27384700
C	4.09776300	0.10244500	-2.32959100

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C	-0.73221700	-2.54159700	-3.94132200
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C	-2.02186100	-2.57594500	-3.39821000
C	2.54123900	-0.73397400	-3.94194200
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H	2.26535700	-4.08786300	-3.96410800
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C	6.15159300	-2.28502900	1.12230600
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C	-1.37118600	-5.05572400	-0.58204200	N	-5.78540400	0.37942900	-0.07059300
C	-0.91953800	-6.48067500	1.00078200	N	-5.24996800	2.53910800	0.10628700
C	-2.29153900	-6.14717100	1.12383900	N	0.37581800	5.78293100	-0.06904400
C	-0.32767800	-7.38396500	1.88525600	N	2.53475300	5.24545200	0.11085000
C	-3.10641200	-6.69595500	2.11977700	H	4.78574100	-3.40473000	-0.11277000
C	-1.13727800	-7.93830400	2.88596700	H	-3.40940100	-4.78213800	-0.11379700
H	0.72052300	-7.64413600	1.79669900	H	-4.78284400	3.40936300	-0.11852500
C	-2.50835600	-7.59338800	2.99497200	H	3.40493300	4.77763400	-0.11282900
H	-4.15593700	-6.43484600	2.20745400	H	5.36065800	0.81683400	-1.04087900
C	-5.05519600	1.37079700	-0.58574200	H	3.99138000	2.66112700	-1.79994400
C	-6.47950000	0.91893100	0.99759900	H	2.66636500	-3.99226400	-1.79557200
C	-6.14684900	2.29119500	1.11999200	H	0.81237600	-5.36046200	-1.03646700
C	-7.38226700	0.32688100	1.88247700	H	-3.99440400	-2.66437300	-1.80115300
C	-6.69608500	3.10618500	2.11558200	H	-5.35870700	-0.81350600	-1.04003500
C	-7.93703300	1.13659100	2.88286700	H	-2.66260300	3.99324200	-1.80356000
H	-7.64178000	-0.72152000	1.79440000	H	-0.81718900	5.35491400	-1.03892500
C	-7.59299700	2.50794200	2.99118200	H	8.05598200	-3.08384600	3.78324300
H	-6.43571600	4.15593900	2.20270700	H	-3.09395700	-8.04835100	3.78600300
C	1.36733300	5.05215300	-0.58311000	H	-8.04827700	3.09364400	3.78195700
C	0.91426400	6.47575900	1.00049900	H	3.08588600	8.04017000	3.78974400
C	2.28602900	6.14177100	1.12484300	C	-0.59110800	-8.90549500	3.86751500
C	0.32162700	7.37837900	1.88513300	O	-1.23197100	-9.43405900	4.76352100
C	3.09990500	6.68939300	2.12223100	O	0.72624900	-9.17120800	3.69007100
C	1.13022100	7.93154200	2.88731700	H	0.98717600	-9.81090700	4.37699800
H	-0.72640200	7.63891200	1.79560100	C	8.91239100	-0.58061400	3.86102200
C	2.50107100	7.58613200	2.99760000	O	9.44236500	-1.22039200	4.75696900
H	4.14926700	6.42794500	2.21086200	O	9.17636800	0.73698100	3.68273600

H	9.81664900	0.99891200	4.36873900
C	0.58318300	8.89790200	3.86919800
O	1.22291400	9.42459400	4.76711000
O	-0.73374200	9.16465600	3.69011300
H	-0.99537700	9.80341100	4.37765000
C	-8.90378400	0.59028600	3.86477300
O	-9.43255000	1.23123800	4.76059300
O	-9.16841900	-0.72741300	3.68824300
H	-9.80778900	-0.98842300	4.37544600

6a



Energy = -4016.3882 Hartree

Number of imaginary frequencies 0

Symbol	X	Y	Z
O	2.28483400	-4.39894400	-1.81930300
O	-4.21962000	2.50805700	-1.65370700
O	-4.40238300	-2.28318800	-1.82075700
O	-2.50675600	-4.21798800	-1.64877400
O	2.50774300	4.21477600	-1.65053600
O	-2.28386800	4.39593000	-1.81821900
O	4.40169900	2.28437000	-1.82280800
O	4.22058900	-2.50678700	-1.65265800
C	-1.33767600	-2.98960900	-3.37562800
C	2.64300800	-0.09544600	-3.92145400
H	1.99561700	-0.08323900	-4.79491300
C	-1.12516700	3.08320000	-3.40908300
C	-2.61517200	-2.44388300	-4.00390300
H	-3.41620100	-3.18804000	-3.94694000
H	-2.41896000	-2.28486700	-5.06825200
C	-1.09237600	3.94919300	-2.30892400
C	-2.98989900	1.33747100	-3.37839200
C	1.09302500	-3.95063000	-2.30816500
C	-0.09541000	-2.64322200	-3.91983500
H	-0.08335800	-1.99756200	-4.79456700
C	-3.83378100	1.34635900	-2.25752600
C	-3.95323900	-1.09207600	-2.31022300

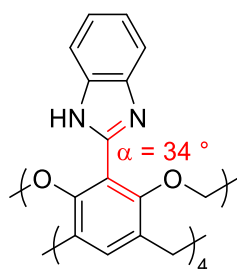
C	3.95319000	1.09268700	-2.31167600
C	0.09530300	2.64240400	-3.92179900
H	0.08281200	1.99694500	-4.79669200
C	-1.34550500	-3.83175700	-2.25335600
C	2.99023700	-1.33781900	-3.37814400
C	1.33768400	2.98838700	-3.37786900
C	-2.64267800	0.09464000	-3.92075900
H	-1.99526700	0.08171700	-4.79420200
C	0.13803700	4.34396100	-1.71649800
C	2.44311700	-2.61528100	-4.00544300
H	3.18696100	-3.41662800	-3.94937700
H	2.28290100	-2.41924700	-5.06965600
C	3.08471100	1.12520700	-3.40977500
C	3.83438000	-1.34579700	-2.25736500
C	4.34935100	-0.13766600	-1.72006400
C	-3.08452300	-1.12558100	-3.40821100
C	-2.44293900	2.61453100	-4.00645400
H	-3.18670000	3.41595900	-3.95009700
H	-2.28321200	2.41841000	-5.07072100
C	-0.13714200	-4.34555300	-1.71531200
C	1.12539900	-3.08396800	-3.40778500
C	2.61504300	2.44290600	-4.00630700
H	3.41585600	3.18728600	-3.94957200
H	2.41890200	2.28352200	-5.07062000
C	1.34606400	3.82999500	-2.25518800
C	-4.34900100	0.13882500	-1.71934600
C	-5.24693600	0.10546300	-0.57149900
C	-6.53134200	-0.67341500	1.00093800
C	-6.53787100	0.74093100	1.12449100
C	-7.27089600	-1.46535800	1.87715600
C	-7.27287700	1.40317300	2.11391300



C	-7.99877200	-0.78958400	2.85776900	N	-5.72062600	1.19473500	0.11868700
H	-7.28440100	-2.54546000	1.80491600	N	-5.72145400	-1.03157900	-0.05920400
C	-8.01047800	0.61553000	2.98749000	N	-1.03359300	5.71083300	-0.05214200
H	-7.27100700	2.48421800	2.20094400	N	1.19274600	5.71246200	0.12417600
C	0.10370100	5.23918500	-0.56651500	N	5.72128500	1.03423200	-0.06033400
C	-0.67566300	6.51825100	1.00998700	N	5.72091700	-1.19198600	0.11846200
C	0.73875900	6.52630800	1.13253000	N	1.03481700	-5.71282100	-0.05136600
C	-1.46780000	7.25423000	1.88902100	N	-1.19139300	-5.71469600	0.12489800
C	1.40096100	7.25943700	2.12341800	H	-5.47570800	2.15211800	-0.10671100
C	-0.79218700	7.97979200	2.87146400	H	2.15015000	5.46933900	-0.10284700
H	-2.54796300	7.26642400	1.81793700	H	5.47613500	-2.14939500	-0.10685700
C	0.61303200	7.99337500	2.99987500	H	-2.14870600	-5.47115500	-0.10197700
H	2.48207900	7.25866800	2.20956000	H	-5.01126300	-2.09442100	-1.02988600
C	5.24725600	-0.10315400	-0.57229800	H	-3.22896700	-3.55881900	-1.78170100
C	6.53032200	0.67666500	1.00073800	H	-3.55996600	3.22964500	-1.78679600
C	6.53725600	-0.73765800	1.12472000	H	-2.09560400	5.00212400	-1.02541700
C	7.26889000	1.46907100	1.87740100	H	3.22930200	3.55529300	-1.78452700
C	7.27158700	-1.39940300	2.11496500	H	5.01058200	2.09639200	-1.03197700
C	7.99605000	0.79376100	2.85890500	H	3.56099000	-3.22873500	-1.78472600
H	7.28217200	2.54915300	1.80487300	H	2.09718300	-5.00770600	-1.02821400
C	8.00823100	-0.61130900	2.98894100	H	-8.59905800	1.07154900	3.77316200
H	7.26983000	-2.48041800	2.20236000	H	1.06881900	8.58016300	3.78701200
C	-0.10250800	-5.24116100	-0.56568000	H	8.59616000	-1.06688600	3.77535500
C	0.67706500	-6.52073400	1.01048500	H	-1.06718600	-8.58444400	3.78619300
C	-0.73734300	-6.52910200	1.13284300	N	-1.58220700	8.76505300	3.81602100
C	1.46932400	-7.25685500	1.88930700	O	-0.98689700	9.41669500	4.68341700
C	-1.39941100	-7.26290400	2.12329100	O	-2.81520500	8.74929000	3.70895600
C	0.79380900	-7.98317000	2.87127200	N	8.78494000	1.58369600	3.80046800
H	2.54947500	-7.26894200	1.81813500	O	9.43601900	0.98842000	4.66831500
C	-0.61142000	-7.99710900	2.99947000	O	8.76820300	2.81673100	3.69411900
H	-2.48054500	-7.26254200	2.20923400	N	1.58390400	-8.76866100	3.81559100

O 0.98872400 -9.41952300 4.68365500  
O 2.81705600 -8.74978100 3.71091100  
N -8.78896800 -1.57908000 3.79863000  
O -9.44175300 -0.98345500 4.66493400  
O -8.77252000 -2.81212200 3.69256300

7a



Energy = -3350.557 Hartree

Number of imaginary frequencies 0

Symbol X Y Z

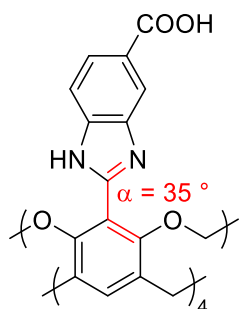
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 O 4.07033400 2.44486900 -1.13504000  
 O -0.17297000 4.73828500 -1.16344700  
 O -2.44493700 4.07022700 -1.13520600  
 O 2.44501200 -4.07035600 -1.13416600  
 O 4.73845600 0.17292400 -1.16294800  
 O 0.17306400 -4.73846400 -1.16224800  
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 C 4.26260700 1.24597500 -0.37347100  
 H 3.33788400 0.97323100 0.14004400  
 H 5.05907800 1.47724100 0.33252500  
 C -1.24594100 4.26253200 -0.37380500  
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 H -0.97316400 3.33784700 0.13976100  
 C 1.24602600 -4.26250400 -0.37271400  
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 H -3.33781000 -0.97306700 0.14033000  
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 C -2.04541400 2.51024800 -2.92327600  
 C -1.27682500 -2.33818500 -3.51077200

H -1.02108000 -1.86350900 -4.45465900  
 C 3.20781100 -0.35707400 -2.92266100  
 C -1.01135200 3.43448700 -3.54213800  
 H -1.31245200 4.47675500 -3.40525400  
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 C 3.81218000 -0.69584100 -1.70432500  
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 H -1.86295000 1.02064000 -4.45499700  
 C 2.82811200 2.66810100 -1.70933100  
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 H 1.02111400 1.86248900 -4.45513600  
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 H 4.47712800 1.31211100 -3.40496600  
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C	-3.56486900	1.93659400	-1.07419200	H	-0.77522100	-5.54796300	3.75190000
C	-3.20774600	0.35645500	-2.92270900	C	-4.15140800	-6.19665300	3.82614000
C	1.01140100	-3.43526400	-3.54130800	H	-5.58840300	-5.75225800	2.26252400
H	1.31251400	-4.47749400	-3.40416700	C	-4.21414100	2.28307100	0.20618600
H	0.95442000	-3.23539700	-4.61474700	C	-5.09609400	2.19439300	2.17334700
C	2.66832800	-2.82822900	-1.70862900	C	-5.16105300	3.55222400	1.77089000
C	1.93670400	3.56468800	-1.07438600	C	-5.59343700	1.81197700	3.42962500
C	2.28318400	4.21401100	0.20595000	C	-5.70986100	4.55182900	2.58150500
C	2.19461500	5.09600200	2.17308400	C	-6.14068800	2.80195100	4.24261100
C	3.55249300	5.16058600	1.77071900	H	-5.54872800	0.77536500	3.75090100
C	1.81224200	5.59351400	3.42930900	C	-6.19810300	4.15143200	3.82465300
C	4.55218500	5.70917400	2.58137800	H	-5.75370200	5.58834500	2.26096200
C	2.80229900	6.14056400	4.24232800	N	3.57138600	4.59260000	0.51581700
H	0.77560000	5.54907500	3.75052100	N	1.43283600	4.50492800	1.17968600
C	4.15182400	6.19760000	3.82446400	N	4.50483000	-1.43250000	1.18037000
H	5.58873600	5.75272000	2.26091000	N	4.59265600	-3.57114600	0.51683000
C	4.21404700	-2.28300600	0.20673300	N	-1.43261400	-4.50451700	1.18081800
C	5.09581900	-2.19411000	2.17395000	N	-3.57118300	-4.59247300	0.51705700
C	5.16049800	-3.55204600	1.77179500	N	-4.50492500	1.43269600	1.17994200
C	5.59317500	-1.81153100	3.43017300	N	-4.59315000	3.57117500	0.51595100
C	5.70903000	-4.55159600	2.58266600	H	4.38469300	4.40233800	-0.05398200
C	6.14016800	-2.80144700	4.24340400	H	4.40248900	-4.38454600	-0.05286800
H	5.54866200	-0.77484200	3.75122600	H	-4.38452300	-4.40240700	-0.05275800
C	6.19729900	-4.15103200	3.82574900	H	-4.40317200	4.38448300	-0.05393300
H	5.75264900	-5.58819400	2.26235800	H	4.89418300	6.63214100	4.48788900
C	-2.28301900	-4.21386900	0.20705200	H	-6.63280000	4.89372300	4.48804800
C	-2.19432200	-5.09537300	2.17440200	H	-4.89371700	-6.63106200	4.48970500
C	-3.55221100	-5.16013700	1.77210400	H	6.63179000	-4.89327600	4.48933400
C	-1.81187300	-5.59254100	3.43073900	H	-2.53532300	-6.53151300	5.22137700
C	-4.55184200	-5.70857200	2.58294200	H	-6.53291300	2.53542900	5.21999700
C	-2.80187000	-6.13943500	4.24393800	H	2.53581100	6.53290800	5.21967600

H 6.53239100 -2.53479800 5.22075600

8a



Energy = -4104.9306 Hartree

Number of imaginary frequencies 0

Symbol	X	Y	Z
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O	3.86352300	2.74635200	-2.03025500
O	2.05661000	4.27617700	-1.99619700
O	-2.05683000	-4.27640000	-1.99560600
O	2.74651800	-3.86366800	-2.02984100
O	-3.86367500	-2.74646200	-2.02983200
O	-4.27669900	2.05684500	-1.99634200
C	3.38003800	-2.87817400	-1.23708200
H	2.64307000	-2.25615100	-0.72383400
H	4.01088300	-3.41741100	-0.53152200
C	2.87801400	3.37950400	-1.23726600
H	3.41712900	4.01027400	-0.53154300
H	2.25606200	2.64233700	-0.72421500
C	-2.87822400	-3.37967900	-1.23678000
H	-2.25632100	-2.64251000	-0.72367100
H	-3.41747400	-4.01038400	-0.53110300
C	-3.38010100	2.87824400	-1.23737800
H	-2.64305500	2.25638600	-0.72401900
H	-4.01092000	3.41765600	-0.53192700
C	0.97594700	3.08814600	-3.79068800
C	-2.65808200	-0.21622200	-4.38021600

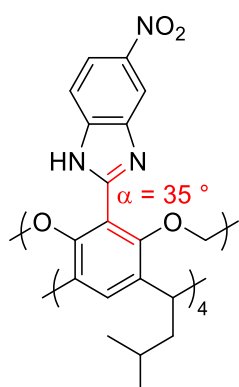
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C	1.46363100	-2.87832400	-3.79231900
C	2.31623300	2.73206100	-4.41063600
H	3.02222600	3.55571900	-4.27294600
H	2.18035000	2.57635300	-5.48426300
C	1.51289400	-3.56765000	-2.57323600
C	3.08839200	-0.97630600	-3.79062000
C	-1.51305900	3.56741000	-2.57375300
C	-0.21616400	2.65770900	-4.38041700
H	-0.16918200	2.12353200	-5.32616300
C	3.78169200	-0.89889000	-2.57561500
C	3.56764100	1.51273400	-2.57375300
C	-3.56773300	-1.51290600	-2.57340600
C	0.21598200	-2.65818400	-4.37995700
H	0.16899300	-2.12411500	-5.32576600
C	0.89854200	3.78125600	-2.57557000
C	-3.08856800	0.97597200	-3.79067000
C	-0.97615100	-3.08851100	-3.79018900
C	2.65790700	0.21581100	-4.38032800
H	2.12360700	0.16879700	-5.32600200
C	0.33971400	-4.04204400	-1.94341500
C	-2.73240100	2.31618900	-4.41073800
H	-3.55601000	3.02225200	-4.27315600
H	-2.57660600	2.18023800	-5.48434500
C	-2.87822300	-1.46378200	-3.79238800
C	-3.78176700	0.89871500	-2.57558300
C	-4.04232400	-0.33966900	-1.94385600
C	2.87808600	1.46346600	-3.79270000
C	2.73220700	-2.31663400	-4.41042800
H	3.55584100	-3.02266000	-4.27274400
H	2.57639800	-2.18086900	-5.48405500

C	-0.33986600	4.04172900	-1.94386300	H	-5.06706300	-2.39945100	2.86482300
C	-1.46379700	2.87797300	-3.79277200	C	-7.48553800	0.05261000	2.93024600
C	-2.31641300	-2.73244500	-4.41019800	H	-7.90359100	1.49256900	1.37353200
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H	-2.18052400	-2.57680900	-5.48383400	C	-0.96896800	5.47142600	1.29574900
C	-0.89877200	-3.78155500	-2.57503000	C	0.12729500	6.27477600	0.88834200
C	4.04230200	0.33959400	-1.94408000	C	-1.56480500	5.67577300	2.54318200
C	4.77591900	0.40916100	-0.66527800	C	0.65428400	7.29094000	1.69608900
C	5.47270800	0.96855000	1.29531900	C	-1.04508600	6.68958300	3.35860700
C	6.27649200	-0.12716500	0.88727300	H	-2.40120600	5.06577500	2.86396800
C	5.67728600	1.56417700	2.54279300	C	0.05164700	7.48328600	2.93143200
C	7.29321400	-0.65396900	1.69452800	H	1.49297900	7.90083600	1.37590400
C	6.69126300	1.04437200	3.35786300	N	5.80809400	-0.45719800	-0.35866800
H	5.06721400	2.40039700	2.86414600	N	4.55103200	1.27511100	0.30883100
C	7.48551400	-0.05182700	2.93010600	N	1.27519600	-4.55011400	0.30966600
H	7.90340000	-1.49221900	1.37374500	N	-0.45702600	-5.80745400	-0.35747700
C	0.40925100	-4.77529800	-0.66437700	N	-4.55104600	-1.27477100	0.30921500
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C	1.04425700	-6.68913700	3.35953000	H	-1.23474300	-6.10338900	-0.93294200
H	2.40028800	-5.06525200	2.86527700	H	-6.10390200	1.23497500	-0.93436500
C	-0.05184900	-7.48361900	2.93196600	H	1.23622500	6.10133500	-0.93246600
H	-1.49209400	-7.90216000	1.37564700	H	8.25934900	-0.41908900	3.59535800
C	-4.77593300	-0.40899900	-0.66505200	H	0.41890800	8.25706200	3.59669600
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C	-6.27656200	0.12755000	0.88736900	H	-0.41914900	-8.25720500	3.59748900
C	-5.67718800	-1.56333800	2.54329500	C	-1.61959700	6.97102800	4.69481000
C	-7.29331800	0.65446000	1.69451400	O	-1.21701700	7.82878700	5.46702800
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H	-2.96099000	6.42638600	5.90786900
C	-6.97144200	-1.61695600	4.69479500
O	-7.83421000	-1.21949800	5.46411700
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H	-6.43028700	-2.96259800	5.90502100
C	1.61804400	-6.96895700	4.69605100
O	1.22063700	-7.83137200	5.46579400
O	2.66311200	-6.16613700	5.01684300
H	2.96374600	-6.42722300	5.90595200
C	6.97168000	1.61831100	4.69419600
O	7.83424600	1.22079400	5.46371400
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9



Energy = -4797.6826 Hartree

Number of imaginary frequencies 0

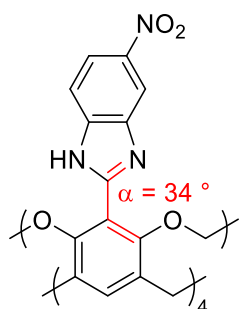
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C	2.89351622	3.36118180	-0.02383752
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C	3.36118180	-2.89351622	-0.02383752
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H	3.99091616	-3.43454841	0.68110610
C	-2.89351622	-3.36118180	-0.02383752
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H	-3.43454841	-3.99091616	0.68110610

C	-3.06903245	0.99336682	-2.58228851
C	0.20335145	-2.63592665	-3.16160135
H	0.16111881	-2.09167056	-4.09816002
C	2.87785597	1.45312826	-2.58461055
C	-2.75803826	2.36017901	-3.19670437
H	-3.54746897	3.03081329	-2.85184933
C	3.56848007	1.49411362	-1.36470937
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C	-2.63592665	-0.20335145	-3.16160135
H	-2.09167056	-0.16111881	-4.09816002
C	0.91806899	3.76551609	-1.36727304
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C	2.63592665	0.20335145	-3.16160135
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C	-3.76551609	0.91806899	-1.36727304
C	-0.99336682	-3.06903245	-2.58228851
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H	-0.16111881	2.09167056	-4.09816002
C	4.03041111	0.31706771	-0.73375478
C	-2.36017901	-2.75803826	-3.19670437
H	-3.03081329	-3.54746897	-2.85184933
C	1.45312826	-2.87785597	-2.58461055
C	-0.91806899	-3.76551609	-1.36727304
C	0.31706771	-4.03041111	-0.73375478
C	-1.45312826	2.87785597	-2.58461055
C	2.36017901	2.75803826	-3.19670437
H	3.03081329	3.54746897	-2.85184933
C	-4.03041111	-0.31706771	-0.73375478

C	-2.87785597	-1.45312826	-2.58461055	H	-1.54309917	-7.88554356	2.57233588
C	2.75803826	-2.36017901	-3.19670437	C	-4.76450728	-0.38051255	0.54497771
H	3.54746897	-3.03081329	-2.85184933	C	-5.46886753	-0.93662126	2.50204067
C	3.76551609	-0.91806899	-1.36727304	C	-6.26657503	0.16593078	2.09242004
C	-0.31706771	4.03041111	-0.73375478	C	-5.68029882	-1.53441283	3.74464161
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C	-1.53441283	5.68029882	3.74464161	C	-7.49197089	0.10316213	4.12920880
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C	-0.99336682	6.69706194	4.53219221	N	0.49195449	5.79404282	0.85044095
H	-2.37559191	5.08873586	4.08378528	N	-1.24850629	4.54796910	1.51862386
C	0.10316213	7.49197089	4.12920880	N	4.54796910	1.24850629	1.51862386
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C	4.76450728	0.38051255	0.54497771	N	1.24850629	-4.54796910	1.51862386
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C	6.69706194	0.99336682	4.53219221	H	6.08768460	-1.26983105	0.27339938
H	5.08873586	2.37559191	4.08378528	H	-1.26983105	-6.08768460	0.27339938
C	7.49197089	-0.10316213	4.12920880	H	-6.08768460	1.26983105	0.27339938
H	7.88554356	-1.54309917	2.57233588	H	0.47115969	8.26328203	4.79351368
C	0.38051255	-4.76450728	0.54497771	H	-8.26328203	0.47115969	4.79351368
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C	1.53441283	-5.68029882	3.74464161	N	-6.95400740	-1.59176786	5.83785997
C	-0.70027293	-7.28335551	2.89452746	O	-7.85855621	-1.11647146	6.53722745
C	0.99336682	-6.69706194	4.53219221	O	-6.25837617	-2.55165661	6.19489729
H	2.37559191	-5.08873586	4.08378528	N	1.59176786	-6.95400740	5.83785997
C	-0.10316213	-7.49197089	4.12920880	O	1.11647146	-7.85855621	6.53722745

O	2.55165661	-6.25837617	6.19489729	C	-3.59695623	-2.57489916	-6.92434399
N	6.95400740	1.59176786	5.83785997	H	-4.27258858	-1.83413621	-5.02961880
O	7.85855621	1.11647146	6.53722745	H	-4.82571934	-4.04377825	-4.00305466
O	6.25837617	2.55165661	6.19489729	H	-5.58677695	-3.88894150	-5.58727570
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O	-1.11647146	7.85855621	6.53722745	H	-3.01927411	-1.67904648	-7.18214550
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9a



Energy = -4168.6208 Hartree

Number of imaginary frequencies 0

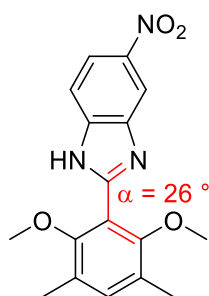
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C	-2.43136500	-3.71661300	-1.21274900
H	-1.90637300	-2.90865700	-0.69779300
H	-2.88715400	-4.41095500	-0.50834800
C	3.71684400	-2.43149000	-1.21290400
H	4.41125000	-2.88732500	-0.50859500
H	2.90895600	-1.90650200	-0.69784000
C	-3.71677200	2.43144700	-1.21284100
H	-2.90887500	1.90644100	-0.69780700
H	-4.41116100	2.88726800	-0.50850600
C	2.43141300	3.71664500	-1.21272100
H	1.90641100	2.90870900	-0.69774500
H	2.88722000	4.41099400	-0.50833800
C	3.18612900	-0.58055800	-3.76474000
C	-0.54828500	2.60719400	-4.35156800

H	-0.43441900	2.08109300	-5.29591500
C	-2.67041000	-1.81350600	-3.76430600
C	3.00096400	-1.95500500	-4.38417100
H	3.90656800	-2.55204100	-4.24706200
H	2.82799400	-1.84049900	-5.45756600
C	-3.34893200	-1.94897900	-2.54607800
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C	3.34895200	1.94898000	-2.54604800
C	2.60719700	0.54832100	-4.35159800
H	2.08107100	0.43449200	-5.29593600
C	-0.41726600	-3.86559400	-2.55102800
C	1.94907400	-3.34894000	-2.54613800
C	-1.94902000	3.34893100	-2.54607800
C	-2.60717100	-0.54829200	-4.35159700
H	-2.08103700	-0.43444400	-5.29592700
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C	0.54832900	-2.60715900	-4.35160300
H	0.43445600	-2.08104900	-5.29594400
C	-3.96774000	-0.84362800	-1.91836400
C	1.95503500	3.00095100	-4.38404600
H	2.55207400	3.90654600	-4.24688400
H	1.84055100	2.82803100	-5.45745000
C	-1.81351600	2.67043100	-3.76431400
C	0.41731500	3.86562400	-2.55099100
C	-0.84367400	3.96768100	-1.91829400
C	1.81356400	-2.67041600	-3.76435900
C	-1.95498900	-3.00092000	-4.38407800
H	-2.55201600	-3.90652600	-4.24692500
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C	1.00400100	-4.68896100	-0.64129300	C	7.31957500	0.25308100	1.71391800
C	1.65419900	-5.31881000	1.31171200	C	6.52878100	1.87218100	3.34133700
C	0.65434800	-6.24520700	0.90928300	H	4.76429400	3.04532300	2.88443500
C	2.28080100	-5.45409200	2.55062200	C	7.45233400	0.87872600	2.94505700
C	0.25318200	-7.31916000	1.71427600	H	8.02057200	-0.51127300	1.39645600
C	1.87252000	-6.52833500	3.34144300	N	0.26438000	-5.81637600	-0.33016100
H	3.04575300	-4.76400900	2.88423000	N	1.84586600	-4.36778300	0.32628600
C	0.87890900	-7.45182300	2.94539500	N	-4.36776900	-1.84562100	0.32636600
H	-0.51125800	-8.02013300	1.39696700	N	-5.81651300	-0.26435300	-0.33026200
C	-4.68901300	-1.00387800	-0.64130000	N	-1.84569500	4.36760000	0.32644600
C	-5.31883200	-1.65395000	1.31176100	N	-0.26449400	5.81643700	-0.33014200
C	-6.24532700	-0.65424100	0.90920800	N	4.36791900	1.84564100	0.32637800
C	-5.45405000	-2.28040400	2.55075600	N	5.81657000	0.26431800	-0.33032000
C	-7.31934300	-0.25310600	1.71412500	H	-0.47495300	-6.20434000	-0.90287000
C	-6.52828300	-1.87205800	3.34156500	H	-6.20454000	0.47487500	-0.90305700
H	-4.76386800	-3.04521500	2.88448300	H	0.47470900	6.20452500	-0.90293000
C	-7.45194200	-0.87868300	2.94532400	H	6.20455400	-0.47491300	-0.90314000
H	-8.02039600	0.51121700	1.39671100	H	0.61159700	-8.26152300	3.61238000
C	-1.00396300	4.68890900	-0.64121000	H	8.26213900	0.61142900	3.61191000
C	-1.65408700	5.31866000	1.31185600	H	-0.61173100	8.26155700	3.61238700
C	-0.65441200	6.24520600	0.90933500	H	-8.26166700	-0.61135800	3.61226800
C	-2.28058200	5.45384100	2.55083500	N	6.70943800	2.50587900	4.64348800
C	-0.25334700	7.31923400	1.71427000	O	7.66439000	2.14946900	5.34607500
C	-1.87234500	6.52811800	3.34164100	O	5.90171600	3.37615900	4.99358800

N	-2.50605200	6.70852700	4.64389500
O	-2.15057300	7.66406000	5.34622800
O	-3.37709800	5.90135900	4.99351000
N	-6.70866900	-2.50565200	4.64387600
O	-7.66463500	-2.15065100	5.34586400
O	-5.90190600	-3.37717200	4.99324700
N	2.50640600	-6.70887600	4.64355300
O	2.14875000	-7.66265800	5.34712400
O	3.37564900	-5.90022900	4.99418600

10



Energy = -918.67491 Hartree

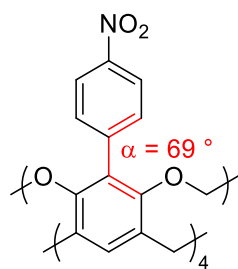
Number of imaginary frequencies 0

Symbol	X	Y	Z
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C	3.96678400	-1.00321900	-0.00611000
C	4.53653900	0.27106700	-0.10240100
H	5.62037600	0.35569100	-0.13319800
C	3.77093900	1.43901400	-0.14550800
C	2.37205400	1.32649000	-0.07939100
O	1.65079800	2.49349800	-0.14089200
C	1.73949600	0.05898400	-0.00449800
C	2.56892700	-1.09136300	0.02857000
C	0.26947900	-0.06824700	0.03916200
C	-1.70451600	-0.97955300	0.52783800
C	-1.85122200	0.25549300	-0.16065000
C	-2.80110200	-1.74845200	0.93959700
C	-3.12238900	0.75038900	-0.45318400
C	-4.06409800	-1.25339500	0.64796800
H	-2.67720500	-2.68993100	1.46419700
C	-4.20573900	-0.02534300	-0.03674300
H	-3.26447000	1.68759300	-0.97681000
N	-0.61090500	0.79317500	-0.44561900
N	-0.35333900	-1.15228100	0.64014000
H	0.13967200	-1.95385300	1.01529100
O	1.99192700	-2.34702300	0.14832000
C	4.42283500	2.79529400	-0.25851100

H	4.11387800	3.30904300	-1.17581300
H	4.15200600	3.44957100	0.57711500
H	5.51183400	2.69590600	-0.27253200
C	4.83527700	-2.23566200	0.06631500
H	4.45565700	-2.95000700	0.80302700
H	4.88373600	-2.75844500	-0.89666100
H	5.85794500	-1.96310600	0.34206900
H	-4.95020300	-1.80174500	0.94097600
N	-5.55247600	0.45519000	-0.32252600
O	-6.51566200	-0.23016500	0.04812100
O	-5.68191800	1.52951900	-0.92453000
C	1.15840100	2.99411700	1.11150300
H	0.43336300	2.30835800	1.56116100
H	1.98259000	3.16937400	1.81393100
H	0.66309400	3.94123200	0.88806400
C	1.77420300	-3.04281100	-1.09722300
H	1.05166600	-2.50591700	-1.72209300
H	2.71204600	-3.16561200	-1.64742400
H	1.37468600	-4.02419300	-0.83383000

11



Energy = -3578.05 Hartree

Number of imaginary frequencies 0

Symbol X Y Z

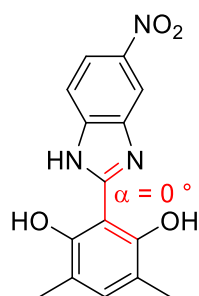
O	-4.25214300	-2.12571400	-1.21993600
O	2.66323900	3.90178000	-1.17863500
O	-2.12571400	4.25214300	-1.21993600
O	-3.90178000	2.66323900	-1.17863500
O	3.90178000	-2.66323900	-1.17863500
O	4.25214300	2.12571400	-1.21993600
O	2.12571400	-4.25214300	-1.21993600
O	-2.66323900	-3.90178000	-1.17863500
C	3.34548200	2.89472600	-0.44093400
H	2.62763400	2.23647800	0.05788300
H	3.96260900	3.43408500	0.27787200
C	-2.89472600	3.34548200	-0.44093400
H	-3.43408500	3.96260900	0.27787200
H	-2.23647800	2.62763400	0.05788300
C	2.89472600	-3.34548200	-0.44093400
H	2.23647800	-2.62763400	0.05788300
H	3.43408500	-3.96260900	0.27787200
C	-3.34548200	-2.89472600	-0.44093400
H	-2.62763400	-2.23647800	0.05788300
H	-3.96260900	-3.43408500	0.27787200
C	-2.89644400	1.42412000	-2.99384600
C	-0.18165500	-2.66045500	-3.58945000

H	-0.14882500	-2.12384200	-4.53437700
C	3.07524500	1.02050800	-3.00953100
C	-2.35709200	2.69787100	-3.62028800
H	-3.07340500	3.51285800	-3.48199100
H	-2.22748500	2.53796900	-4.69419800
C	3.77962800	0.95814600	-1.80013800
C	1.42412000	2.89644400	-2.99384600
C	-3.77962800	-0.95814600	-1.80013800
C	-2.66045500	0.18165500	-3.58945000
H	-2.12384200	0.14882500	-4.53437700
C	1.45069000	3.58672900	-1.77218500
C	-0.95814600	3.77962800	-1.80013800
C	0.95814600	-3.77962800	-1.80013800
C	2.66045500	-0.18165500	-3.58945000
H	2.12384200	-0.14882500	-4.53437700
C	-3.58672900	1.45069000	-1.77218500
C	-1.42412000	-2.89644400	-2.99384600
C	2.89644400	-1.42412000	-2.99384600
C	0.18165500	2.66045500	-3.58945000
H	0.14882500	2.12384200	-4.53437700
C	4.06407900	-0.26924100	-1.17164400
C	-2.69787100	-2.35709200	-3.62028800
H	-3.51285800	-3.07340500	-3.48199100
H	-2.53796900	-2.22748500	-4.69419800
C	1.02050800	-3.07524500	-3.00953100
C	-1.45069000	-3.58672900	-1.77218500
C	-0.26924100	-4.06407900	-1.17164400
C	-1.02050800	3.07524500	-3.00953100
C	2.69787100	2.35709200	-3.62028800
H	3.51285800	3.07340500	-3.48199100
H	2.53796900	2.22748500	-4.69419800



C	-4.06407900	0.26924100	-1.17164400	H	0.29045700	-6.70193800	-0.88909500
C	-3.07524500	-1.02050800	-3.00953100	C	-0.69872900	-5.04176800	2.48244300
C	2.35709200	-2.69787100	-3.62028800	H	-0.90324700	-3.22926900	1.36118400
H	3.07340500	-3.51285800	-3.48199100	C	-0.37387900	-6.39745200	2.41350200
H	2.22748500	-2.53796900	-4.69419800	H	0.23006800	-8.06307300	1.18250900
C	3.58672900	-1.45069000	-1.77218500	H	-0.96911800	-4.59076100	3.42924100
C	0.26924100	4.06407900	-1.17164400	C	-4.86989100	0.30887400	0.08526300
C	0.30887400	4.86989100	0.08526300	C	-6.23720700	-0.01568500	0.05211400
C	0.66340500	4.28640700	1.31311900	C	-4.28640700	0.66340500	1.31311900
C	-0.01568500	6.23720700	0.05211400	C	-7.00867200	0.01568500	1.20988200
C	0.69872900	5.04176800	2.48244300	H	-6.70193800	-0.29045700	-0.88909500
H	0.90324700	3.22926900	1.36118400	C	-5.04176800	0.69872900	2.48244300
C	0.01568500	7.00867200	1.20988200	H	-3.22926900	0.90324700	1.36118400
H	-0.29045700	6.70193800	-0.88909500	C	-6.39745200	0.37387900	2.41350200
C	0.37387900	6.39745200	2.41350200	H	-8.06307300	-0.23006800	1.18250900
H	0.96911800	4.59076100	3.42924100	H	-4.59076100	0.96911800	3.42924100
H	-0.23006800	8.06307300	1.18250900	N	0.40684100	7.19983600	3.63888100
C	4.86989100	-0.30887400	0.08526300	O	0.74692300	6.64752600	4.69112400
C	6.23720700	0.01568500	0.05211400	O	0.09238700	8.39260600	3.56606800
C	4.28640700	-0.66340500	1.31311900	N	7.19983600	-0.40684100	3.63888100
C	7.00867200	-0.01568500	1.20988200	O	8.39260600	-0.09238700	3.56606800
H	6.70193800	0.29045700	-0.88909500	O	6.64752600	-0.74692300	4.69112400
C	5.04176800	-0.69872900	2.48244300	N	-0.40684100	-7.19983600	3.63888100
H	3.22926900	-0.90324700	1.36118400	O	-0.09238700	-8.39260600	3.56606800
C	6.39745200	-0.37387900	2.41350200	O	-0.74692300	-6.64752600	4.69112400
H	8.06307300	0.23006800	1.18250900	N	-7.19983600	0.40684100	3.63888100
H	4.59076100	-0.96911800	3.42924100	O	-8.39260600	0.09238700	3.56606800
C	-0.30887400	-4.86989100	0.08526300	O	-6.64752600	0.74692300	4.69112400
C	0.01568500	-6.23720700	0.05211400				
C	-0.66340500	-4.28640700	1.31311900				
C	-0.01568500	-7.00867200	1.20988200				

S6



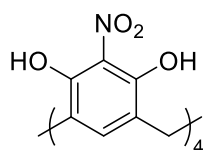
Energy = -840.10356 Hartree

Number of imaginary frequencies 0

Symbol	X	Y	Z
C	-4.18290000	-0.91538700	-0.00008000
C	-4.64892600	0.40787500	-0.00000800
H	-5.72405900	0.57244300	-0.00000300
C	-3.80806200	1.51974600	0.00001300
C	-2.41816800	1.29758800	-0.00002200
O	-1.61916600	2.38550000	0.00001000
C	-1.88729000	-0.02539900	-0.00005100
C	-2.79975000	-1.10881900	-0.00008200
C	-0.44148600	-0.20675900	-0.00003100
C	1.56773300	-1.16704800	0.00005800
C	1.68369100	0.24806600	-0.00002200
C	2.68320900	-2.01175700	0.00013700
C	2.93849500	0.85469600	-0.00003600
C	3.93376800	-1.40829400	0.00012900
H	2.58336300	-3.09172600	0.00019800
C	4.04176300	-0.00120900	0.00004200
H	3.05627500	1.93089500	-0.00009600
N	0.42180400	0.80981500	-0.00007800
N	0.21853400	-1.41629300	0.00006300
H	-0.24180100	-2.31823700	0.00001300
O	-2.26595400	-2.37616600	-0.00021700
C	-4.34640600	2.92763900	0.00008400

H	-4.00854200	3.48820100	0.87976500
H	-4.00824500	3.48840600	-0.87934900
H	-5.44013500	2.91959200	-0.00009400
C	-5.13300100	-2.09034900	-0.00013200
H	-5.01068500	-2.72711200	-0.88724200
H	-5.01105100	-2.72690400	0.88718500
H	-6.16790500	-1.73882700	-0.00036900
H	4.83338800	-2.01010600	0.00018700
H	-0.66759500	2.08000900	0.00000300
H	-2.97278000	-3.03928600	0.00066900
N	5.37619600	0.59091800	0.00003300
O	6.35731600	-0.16441800	0.00023600
O	5.47380700	1.82483900	-0.00015300

S7



Energy = -2501.4659 Hartree

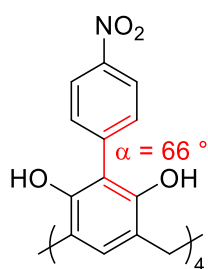
Number of imaginary frequencies 0

Symbol	X	Y	Z
O	2.41007000	-2.45254400	-2.97110000
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O	2.48105000	4.98327200	1.01258400
O	2.46210100	2.41391800	-2.96554300
O	-2.46210200	-2.41391800	-2.96554300
O	-2.41007100	2.45254400	-2.97109900
O	-2.48105000	-4.98327100	1.01258700
O	2.38800300	-5.02821900	1.00662500
O	2.37746800	-1.10001800	-5.11032400
C	2.52977400	1.21466400	-0.94829300
N	0.05824800	6.37179000	1.65472100
C	-0.02583000	-2.60949500	-0.16500200
H	-0.01772900	-1.63396600	-0.63903000
C	-2.50399900	1.25961100	-0.95104500
C	2.60187000	2.51028300	-0.17333800
H	3.23735000	3.22145800	-0.71072200
C	-2.44813100	1.26613000	-2.34980700
O	-1.02069800	6.95230800	1.92638000
C	-1.20522200	3.20649300	0.11941900
C	2.44813000	-1.26613000	-2.34980800
C	2.54688300	-0.02350100	-0.29912700
H	2.60525600	-0.02529000	0.78711800
N	2.41165400	-0.01739200	-4.47792900
C	-1.20170200	4.46488700	0.73016500

N	-2.41165500	0.01739300	-4.47792900
C	1.28519800	4.44198800	0.73327300
O	1.02069800	-6.95231100	1.92637400
C	-1.28519800	-4.44198800	0.73327500
O	1.14707400	6.93092800	1.93164200
C	-2.54688400	0.02350000	-0.29912700
H	-2.60525600	0.02528900	0.78711900
C	2.47555700	1.22547400	-2.34708400
N	-0.05824800	-6.37178900	1.65472300
C	1.20522200	-3.20649400	0.11941900
C	-2.52977500	-1.21466400	-0.94829300
C	0.02582900	2.60949400	-0.16500200
H	0.01772800	1.63396500	-0.63902800
O	-2.37746000	1.10001900	-5.11032300
C	-2.44005200	0.01928300	-3.06333700
C	2.55197300	-2.55803400	-0.17881900
H	3.17216000	-3.28041000	-0.71911800
C	-1.26693700	-3.18392300	0.12223900
C	1.20170200	-4.46488700	0.73016600
C	-0.04729100	-5.09870100	1.04161000
C	1.26693700	3.18392300	0.12223900
C	-2.55197300	2.55803300	-0.17881700
H	-3.17216100	3.28040900	-0.71911600
O	2.41890200	1.06686600	-5.10837400
C	2.44005100	-0.01928300	-3.06333800
C	2.50399800	-1.25961100	-0.95104600
C	-2.60187100	-2.51028400	-0.17333800
H	-3.23735000	-3.22145900	-0.71072200
O	-2.41889400	-1.06686600	-5.10837300
C	-2.47555800	-1.22547400	-2.34708400
C	0.04729100	5.09870200	1.04160700

O -1.14707400 -6.93093100 1.93163600  
H 2.44729300 2.24583000 -3.93793900  
H 2.31929800 5.86258900 1.42975700  
H -2.21102500 5.90495200 1.42307600  
H -2.39048700 2.28164200 -3.94294300  
H -2.44729600 -2.24582900 -3.93793900  
H -2.31929800 -5.86258700 1.42976200  
H 2.21102500 -5.90495000 1.42308100  
H 2.39048400 -2.28164100 -3.94294400  
H -3.06820100 2.37402300 0.77095000  
H 3.11195600 2.31446000 0.77739600  
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S8



Energy = -3425.7431 Hartree

Number of imaginary frequencies 0

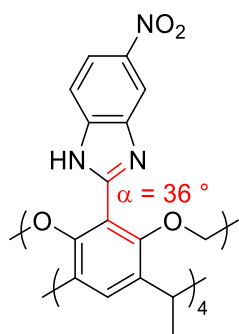
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 O -1.86337200 4.57307800 -1.01246900  
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 C 2.62089700 -0.27966900 -3.26994400  
 H 1.96082200 -0.20160700 -4.13032600  
 C -0.89834700 3.15447800 -2.73645000  
 C -2.79021500 -2.24187000 -3.36055500  
 H -3.64140500 -2.92876100 -3.30899600  
 H -2.60159500 -2.07099300 -4.42481700  
 C -0.78207500 4.01406900 -1.62782400  
 C -2.89582400 1.55209300 -2.76405500  
 C 0.78207500 -4.01406900 -1.62782400  
 C -0.27966900 -2.62089700 -3.26994400  
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 C -3.78079200 1.62792700 -1.68119600  
 C -4.01406900 -0.78207500 -1.62782400

C 4.01406900 0.78207500 -1.62782400  
 C 0.27966900 2.62089700 -3.26994400  
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 C 0.48340700 4.35099200 -1.09904900  
 C 2.24187000 -2.79021500 -3.36055500  
 H 2.92876100 -3.64140500 -3.30899600  
 H 2.07099300 -2.60159500 -4.42481700  
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 H -2.67424600 4.05200700 -1.17614400  
 H -4.70048600 2.85442000 -0.47083000  
 H -4.05200700 -2.67424600 -1.17614400  
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H	4.70048600	-2.85442000	-0.47083000	H	8.54557500	-0.05128000	0.92298400
H	2.85442000	4.70048600	-0.47083000	H	5.33959900	-1.62865400	3.32679500
H	4.05200700	2.67424600	-1.17614400	C	0.60184700	5.28144700	0.06117300
C	-5.28144700	0.60184700	0.06117300	C	0.22129900	6.63138900	-0.05797000
C	-4.82741700	1.11121000	1.29279300	C	1.11121000	4.82741700	1.29279300
C	-6.63138900	0.22129900	-0.05797000	C	0.34243700	7.50650100	1.01600700
C	-5.69208000	1.24302600	2.37816800	H	-0.17077500	6.99731800	-1.00083500
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C	-7.50650100	0.34243700	1.01600700	H	1.38542300	3.78346800	1.41350300
H	-6.99731800	-0.17077500	-1.00083500	C	0.85586000	7.02282800	2.22238800
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C	-0.22129900	-6.63138900	-0.05797000	O	-1.46162600	-7.50104800	4.41204200
C	-1.11121000	-4.82741700	1.29279300	N	-7.94020900	0.98983500	3.35790100
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H	-0.05128000	-8.54557500	0.92298400	N	7.94020900	-0.98983500	3.35790100
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C	4.82741700	-1.11121000	1.29279300				
C	7.50650100	-0.34243700	1.01600700				
H	6.99731800	0.17077500	-1.00083500				
C	5.69208000	-1.24302600	2.37816800				
H	3.78346800	-1.38542300	1.41350300				
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S9



Energy = -4325.8749 Hartree

Number of imaginary frequencies 0

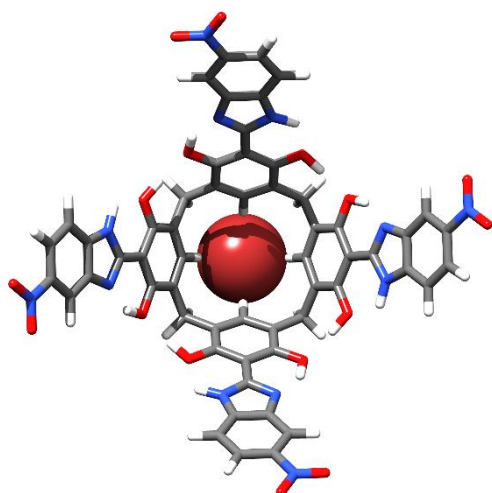
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O	-1.29935981	-4.55305845	-1.68450574
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C	4.43402481	-0.12997653	-0.89658840
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C	-1.16359543	3.01532206	-3.45874402
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H	-1.53778560	-1.44867494	-4.98036089
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C	-3.01532206	-1.16359543	-3.45874402
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H	1.53778560	1.44867494	-4.98036089
C	2.78402651	-2.93356673	-1.60963300
C	-3.62290572	0.09896647	-4.07345707
H	-4.66578534	0.13243979	-3.74814021
C	-1.32140097	-2.93815215	-3.45794767
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C	1.32140097	2.93815215	-3.45794767
C	3.62290572	-0.09896647	-4.07345707
H	4.66578534	-0.13243979	-3.74814021
C	-2.78402651	2.93356673	-1.60963300
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C	-0.09896647	-3.62290572	-4.07345707	C	-3.30052402	3.46897284	-0.33533853
H	-0.13243979	-4.66578534	-3.74814021	C	-4.17389151	3.67429070	1.62139521
C	1.65814559	-3.50709161	-2.24266019	C	-3.84468909	4.98927564	1.19434255
C	2.93356673	2.78402651	-1.60963300	C	-4.76399753	3.46718890	2.86839550
C	3.46897284	3.30052402	-0.33533853	C	-4.08799114	6.12158195	1.98265064
C	3.67429070	4.17389151	1.62139521	C	-5.00236519	4.60352926	3.64196224
C	4.98927564	3.84468909	1.19434255	H	-5.02631306	2.47759636	3.22113991
C	3.46718890	4.76399753	2.86839550	C	-4.67596308	5.91249158	3.22163544
C	6.12158195	4.08799114	1.98265064	H	-3.83206531	7.12078099	1.64658432
C	4.60352926	5.00236519	3.64196224	N	4.82184145	3.29434566	-0.04718587
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C	5.91249158	4.67596308	3.22163544	N	3.82323492	-2.75645345	0.64795057
H	7.12078099	3.83206531	1.64658432	N	3.29434566	-4.82184145	-0.04718587
C	3.30052402	-3.46897284	-0.33533853	N	-2.75645345	-3.82323492	0.64795057
C	4.17389151	-3.67429070	1.62139521	N	-4.82184145	-3.29434566	-0.04718587
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C	4.76399753	-3.46718890	2.86839550	N	-3.29434566	4.82184145	-0.04718587
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H	3.83206531	-7.12078099	1.64658432	H	6.74798409	4.88958805	3.87575925
C	-3.46897284	-3.30052402	-0.33533853	H	-4.88958805	6.74798409	3.87575925
C	-3.67429070	-4.17389151	1.62139521	H	-6.74798409	-4.88958805	3.87575925
C	-4.98927564	-3.84468909	1.19434255	H	4.88958805	-6.74798409	3.87575925
C	-3.46718890	-4.76399753	2.86839550	N	-5.62443887	4.43150210	4.95070867
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H	-2.47759636	-5.02631306	3.22113991	N	-4.43150210	-5.62443887	4.95070867
C	-5.91249158	-4.67596308	3.22163544	O	-5.43846953	-5.84170598	5.63775186
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N 5.62443887 -4.43150210 4.95070867  
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6a-Br<sup>-</sup>



Energy = -6588.2928 Hartree

Number of imaginary frequencies 0

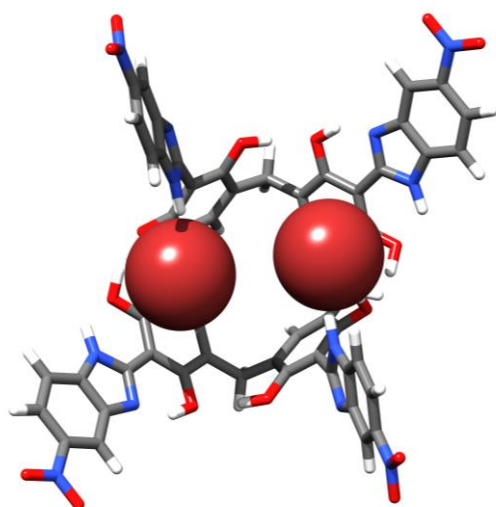
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C	3.01976100	1.26813800	2.99365300
C	0.03233200	-2.64656400	3.53850100
H	0.02992000	-1.97872500	4.40029000
C	-3.06446300	1.19474600	3.02088500
C	2.50037000	2.55944200	3.61989700
H	3.26542000	3.34129900	3.56612200
H	2.33070100	2.36512900	4.68209100
C	-3.93652000	1.17821500	1.92619700
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C	3.93652000	-1.17821500	1.92619700

C	2.64656400	0.03233200	3.53850100
H	1.97872500	0.02992000	4.40029000
C	-1.26257000	3.86366500	1.87475200
C	1.17821500	3.93652000	1.92619700
C	-1.17821500	-3.93652000	1.92619700
C	-2.64656400	-0.03233200	3.53850100
H	-1.97872500	-0.02992000	4.40029000
C	3.86366500	1.26257000	1.87475200
C	1.26813800	-3.01976100	2.99365300
C	-3.01976100	-1.26813800	2.99365300
C	-0.03233200	2.64656400	3.53850100
H	-0.02992000	1.97872500	4.40029000
C	-4.35612200	-0.04521800	1.33464100
C	2.55944200	-2.50037000	3.61989700
H	3.34129900	-3.26542000	3.56612200
H	2.36512900	-2.33070100	4.68209100
C	-1.19474600	-3.06446300	3.02088500
C	1.26257000	-3.86366500	1.87475200
C	0.04521800	-4.35612200	1.33464100
C	1.19474600	3.06446300	3.02088500
C	-2.55944200	2.50037000	3.61989700
H	-3.34129900	3.26542000	3.56612200
H	-2.36512900	2.33070100	4.68209100
C	4.35612200	0.04521800	1.33464100
C	3.06446300	-1.19474600	3.02088500
C	-2.50037000	-2.55944200	3.61989700
H	-3.26542000	-3.34129900	3.56612200
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C	-1.30172600	7.29766800	-2.48078900	H	7.30299700	2.38352000	-2.55916000
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H	2.64873600	7.27998200	-2.20066500	N	1.13849600	5.71963700	-0.32952200
C	-0.51580200	8.03271000	-3.35819900	N	-5.71963700	1.13849600	-0.32952200
H	-2.38352000	7.30299700	-2.55916000	N	-5.73923100	-1.08979400	-0.49350200
C	-5.25349700	0.00000000	0.18910100	N	-1.13849600	-5.71963700	-0.32952200
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C	-7.27374100	1.56802800	-2.26448500	N	5.73923100	1.08979400	-0.49350200
C	-7.29766800	-1.30172600	-2.48078900	H	-2.04638200	5.49938600	-0.25903400
C	-8.01035500	0.89012300	-3.23861000	H	-5.49938600	-2.04638200	-0.25903400
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C	-8.03271000	-0.51580200	-3.35819900	H	5.49938600	2.04638200	-0.25903400
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C	0.63718600	-6.55556000	-1.49833800	H	-4.97649700	2.20297000	0.64784500
C	-1.56802800	-7.27374100	-2.26448500	H	-3.62231700	-3.15256900	1.40484900
C	1.30172600	-7.29766800	-2.48078900	H	-2.20297000	-4.97649700	0.64784500
C	-0.89012300	-8.01035500	-3.23861000	H	3.15256900	-3.62231700	1.40484900
H	-2.64873600	-7.27998200	-2.20066500	H	4.97649700	-2.20297000	0.64784500
C	0.51580200	-8.03271000	-3.35819900	H	-0.97342700	8.62647900	-4.13897900
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C	7.27374100	-1.56802800	-2.26448500	O	-9.45595600	1.08156600	-5.04411100
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6a·(Br<sup>-</sup>)<sub>2</sub>



Energy = -9160.1678 Hartree

Number of imaginary frequencies 0

Symbol X Y Z

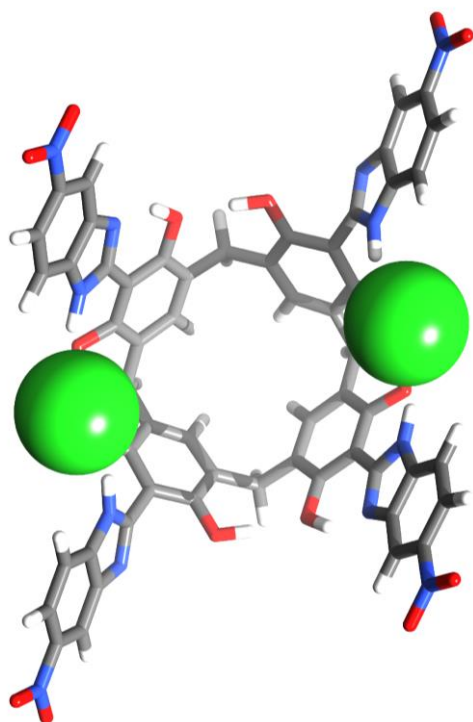
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C	1.93846700	-3.09148700	-4.06504700
H	2.54978500	-3.99539200	-3.97989000
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C	3.57526700	0.36341600	-2.02668300

C	2.59064100	-0.65445900	-3.95338200
H	2.17438200	-0.56321100	-4.95418500
C	-2.09219300	-3.78297600	-2.59356600
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C	-0.27045800	4.38288300	-2.63085700
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H	-0.36047300	-1.79988900	-4.71113000
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C	-3.06641000	-7.66025000	1.23575800	H	4.27093100	0.18264100	3.85037100
C	-1.12295900	-8.95339800	1.89946000	N	-2.43670900	-5.95714200	-0.53138500
H	0.78924000	-8.52556200	0.96756300	N	-0.25944400	-6.43748000	-0.68778700
C	-2.49946200	-8.66133800	2.01250400	N	-5.49449400	1.81180100	0.03458600
H	-4.12257600	-7.42449500	1.30943800	N	-4.01646400	0.44400200	1.03064500
C	-4.41221500	1.06845700	-0.13238800	N	0.25944400	6.43748000	-0.68778700
C	-5.82621700	1.67013900	1.37039000	N	2.43670900	5.95714200	-0.53138500
C	-4.90008900	0.79822900	2.00998000	N	5.49449400	-1.81180100	0.03458600
C	-6.87287000	2.23723400	2.09542000	N	4.01646400	-0.44400200	1.03064500
C	-4.98775700	0.47586300	3.37159300	H	-3.29405700	-5.44772700	-0.71488400
C	-6.95052300	1.90336100	3.45041500	H	-3.22332100	-0.21432200	1.11530700
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C	-6.03158900	1.03956600	4.09008100	H	3.22332100	0.21432200	1.11530700
H	-4.27093100	-0.18264100	3.85037100	H	0.99960900	-5.78479400	-1.51500000
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C	0.83070500	7.26713900	0.25761000	H	-3.78165700	-3.13256800	-1.95402500
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C	3.06641000	7.66025000	1.23575800	H	-0.99960900	5.78479400	-1.51500000
C	1.12295900	8.95339800	1.89946000	H	3.78165700	3.13256800	-1.95402500
H	-0.78924000	8.52556200	0.96756300	H	3.34539800	1.65842000	-0.58204200
C	2.49946200	8.66133800	2.01250400	H	-3.10677000	-9.22774100	2.70666700
H	4.12257600	7.42449500	1.30943800	H	-6.15002600	0.82805400	5.14501200
C	4.41221500	-1.06845700	-0.13238800	H	3.10677000	9.22774100	2.70666700
C	5.82621700	-1.67013900	1.37039000	H	6.15002600	-0.82805400	5.14501200
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C	6.87287000	-2.23723400	2.09542000	O	-8.09624000	2.18797400	5.44761500
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6a·(Cl)<sub>2</sub>



Energy = -4937.1027 Hartree

Number of imaginary frequencies 0

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O	-1.61875500	-4.76346900	-1.62170200
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O	-4.61591200	1.66085900	-1.60052200
C	0.73042600	3.23843200	-3.27923900
C	-2.58062800	-0.42434600	-3.81348300
H	-1.95971700	-0.33264700	-4.70160000
C	1.70027300	-2.84350100	-3.29896000
C	2.09492000	2.91653700	-3.87992300
H	2.75399500	3.78792800	-3.81006200

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C	3.15321200	-0.73786500	-3.28459500
C	-1.84212400	3.74570300	-2.23192600
C	-0.41483600	2.63562500	-3.80404800
H	-0.29828400	1.95704600	-4.64586700
C	3.96250100	-0.60211800	-2.14821000
C	3.59041400	1.80852900	-2.13943000
C	-3.59041400	-1.80852900	-2.13943000
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C	-3.15321200	0.73786500	-3.28459500
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C	0.73037200	-4.45358700	-1.72677300
C	-2.88021600	2.09750600	-3.91212600
H	-3.77983400	2.72093600	-3.87956500
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C	-3.96250100	0.60211800	-2.14821000
C	-4.16786400	-0.65867300	-1.53810600
C	2.77624300	1.69869300	-3.27504000
C	2.88021600	-2.09750600	-3.91212600
H	3.77983400	-2.72093600	-3.87956500
H	2.65945500	-1.94027300	-4.97232300
C	-0.73037200	4.45358700	-1.72677300
C	-1.70027300	2.84350100	-3.29896000
C	-2.09492000	-2.91653700	-3.87992300
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H	-1.94948700	-2.72652300	-4.94792100	C	-0.79469400	7.57938200	0.03082600
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C	4.87819900	0.80418300	-0.27331500	C	-1.86550300	7.26603900	2.24080000
C	5.79774800	1.74215400	1.45548500	C	-1.05184400	9.42959400	1.49747200
C	5.75963300	0.34478500	1.71075500	H	-0.12706900	9.58652800	-0.45785200
C	6.34151300	2.61984900	2.39039300	C	-1.67394500	8.61970500	2.47525400
C	6.25147400	-0.21224500	2.89741000	H	-2.34136400	6.63091500	2.98009900
C	6.83060600	2.04820700	3.56741400	N	5.18239200	-0.21355700	0.59936500
H	6.38229300	3.68818700	2.22000100	N	5.24211500	1.99143100	0.21498500
C	6.79048300	0.66170600	3.83136300	N	0.47197200	-6.82087000	-1.07952400
H	6.21063700	-1.27932000	3.08559900	N	1.44516400	-5.50862800	0.46060100
C	0.87524000	-5.59397400	-0.79333800	N	-5.24211500	-1.99143100	0.21498500
C	0.79469400	-7.57938200	0.03082600	N	-5.18239200	0.21355700	0.59936500
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C	1.86550300	-7.26603900	2.24080000	H	4.92364800	-1.19143100	0.46792000
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C	1.67394500	-8.61970500	2.47525400	H	-1.91175200	4.68872800	0.86761100
H	2.34136400	-6.63091500	2.98009900	H	4.40139000	2.96283300	-0.81620200
C	-4.87819900	-0.80418300	-0.27331500	H	2.42696100	4.21267200	-1.69275800
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C	-6.25147400	0.21224500	2.89741000	H	-4.40139000	-2.96283300	-0.81620200
C	-6.83060600	-2.04820700	3.56741400	H	-4.15712500	2.50722600	-1.79934500
H	-6.38229300	-3.68818700	2.22000100	H	-3.16629700	3.92772900	-0.75341700
C	-6.79048300	-0.66170600	3.83136300	H	7.18373500	0.28880300	4.76828300
H	-6.21063700	1.27932000	3.08559900	H	1.99720000	-9.06693600	3.40643400
C	-0.87524000	5.59397400	-0.79333800	H	-7.18373500	-0.28880300	4.76828300

H	-1.99720000	9.06693600	3.40643400	O	-0.32391000	11.55958800	0.93263900
N	0.87524000	-10.84642100	1.78320000	N	7.41174300	2.92860400	4.57308800
O	1.28465000	-11.28851200	2.86665300	O	7.83549400	2.42819900	5.62440300
O	0.32391000	-11.55958800	0.93263900	O	7.46202000	4.14370500	4.33764400
N	-7.41174300	-2.92860400	4.57308800	Cl	-3.61928900	3.33452900	1.22454800
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O	-7.46202000	-4.14370500	4.33764400				
N	-0.87524000	10.84642100	1.78320000				
O	-1.28465000	11.28851200	2.86665300				

## 6. References

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- <sup>1</sup> S. Miao, R. D. Adams, D.-S. Guo, Q.-F. Zhang, *J. Mol. Struct.*, 2003, **659**, 119 - 128.
- <sup>2</sup> M. Grajda, M. Wierzbicki, P. Cmoch, A. Szumna, *J. Org. Chem.*, 2013, **78**, 11597 - 11601.
- <sup>3</sup> P. Jurek, H. Jędrzejewska, M. R. Rode, A. Szumna, *Chem. Eur. J.*, 2023, **29**, e2022031
- <sup>4</sup> P. Jurek, M. F. Rode, M. P. Szymański, M. Banasiewicz, A. Szumna, *J. Mater. Chem. C*, 2023, **11**, 10642 - 10650.
- <sup>5</sup> M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, GAUSSIAN 16 (Revision C.01) Gaussian Inc., Wallingford, CT, 2016.