

## Self-assembly and recognition properties of a tetraanionic macrocyclic boronate ester in aqueous medium

Mayte A. Martínez-Aguirre, Jorge M. del Campo, Sigfrido Escalante-Tovar and Anatoly K. Yatsimirsky\*

Facultad de Química, Universidad Nacional Autónoma de México, 04510 México D.F., México.  
E-mail: anatoli@unam.mx

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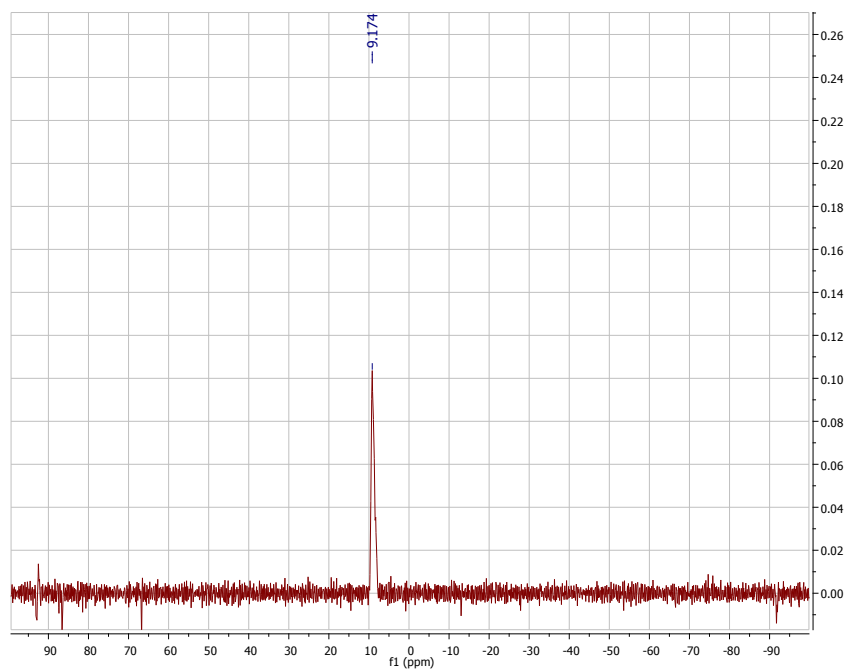


Fig. 1S.  $^{11}\text{B}$  NMR spectrum of **3** prepared by mixing 40 mM **1**, 40 mM **2** and 80 mM NaOH in 5% vol. DMSO- $\text{d}_6/\text{D}_2\text{O}$ .

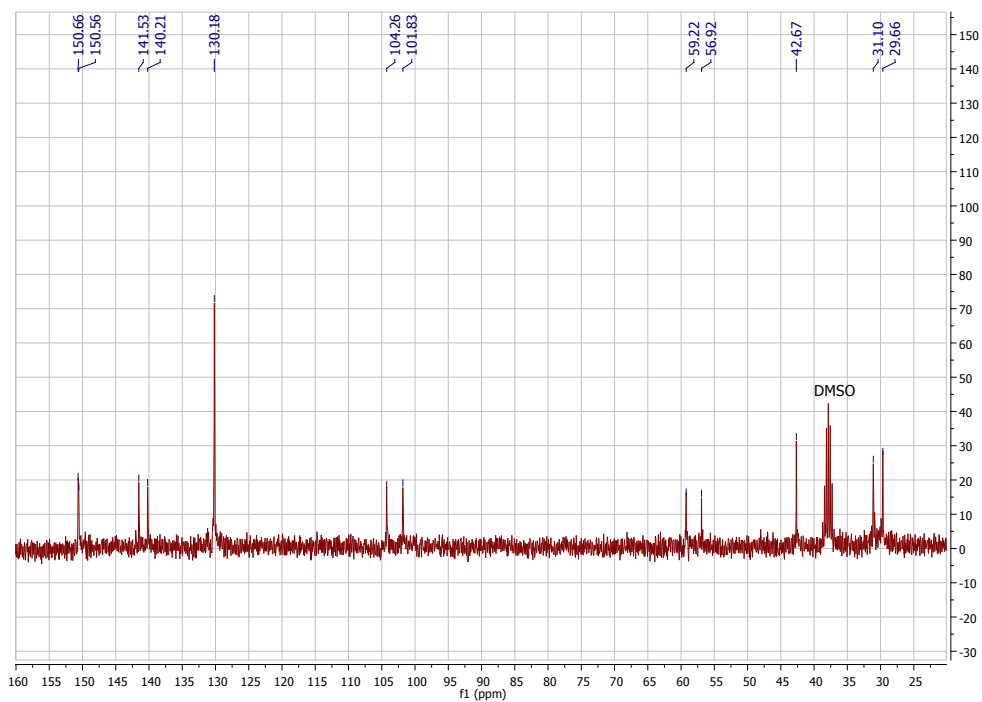


Fig. 2S.  $^{13}\text{C}$  NMR spectrum of **3** prepared by mixing 40 mM **1**, 40 mM **2** and 80 mM NaOH in 5% vol. DMSO- $\text{d}_6/\text{D}_2\text{O}$ .

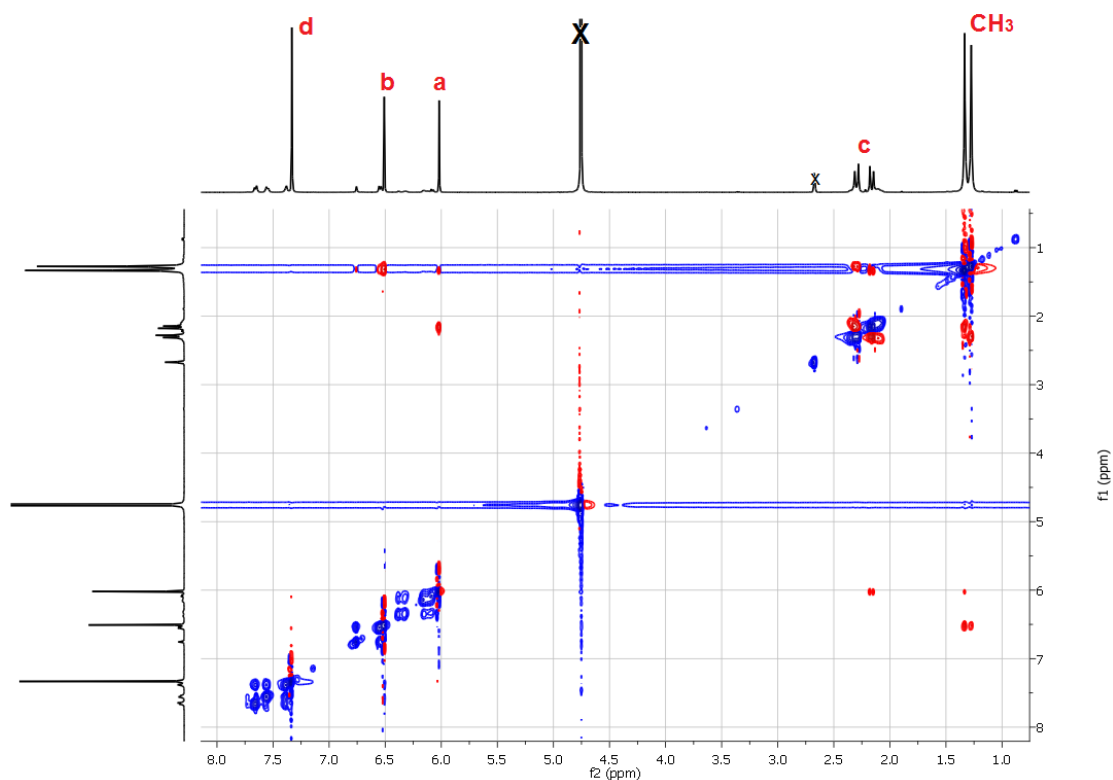


Fig. 3S. ROESY  $^1\text{H}$  spectrum of **3** prepared by mixing 10 mM **1**, 10 mM **2** and 20 mM NaOH in 5% vol. DMSO- $d_6$ /D $_2$ O. Crossed peaks belong to residual solvent signals.

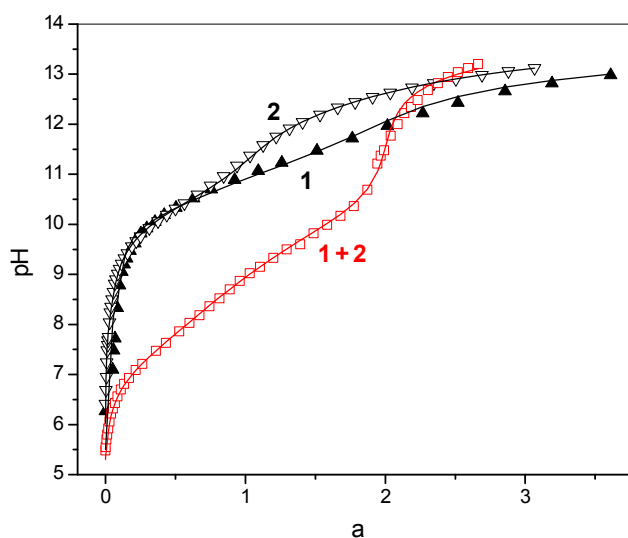
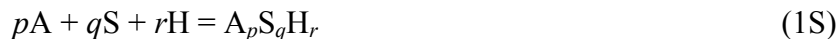


Fig. 4S. Potentiometric titrations of **1** (solid triangles), **2** (open triangles) and the equimolar mixture of **1** and **2** (open red squares) in 50% DMSO/water containing 0.05 M NaCl as a background electrolyte; “a” is the number of equivalents of NaOH. Solid lines are theoretical fitting curves generated by Hyperquad 2003.

The titration results were fitted to a traditional “ $pqr$ ” scheme, reaction (1S), where A is the neutral form of diboronic acid **2** ( $R(B(OH)_2)_2$ ), S is the neutral form of dicatechol **1** ( $R'(OH)_4$ ) and H is proton.

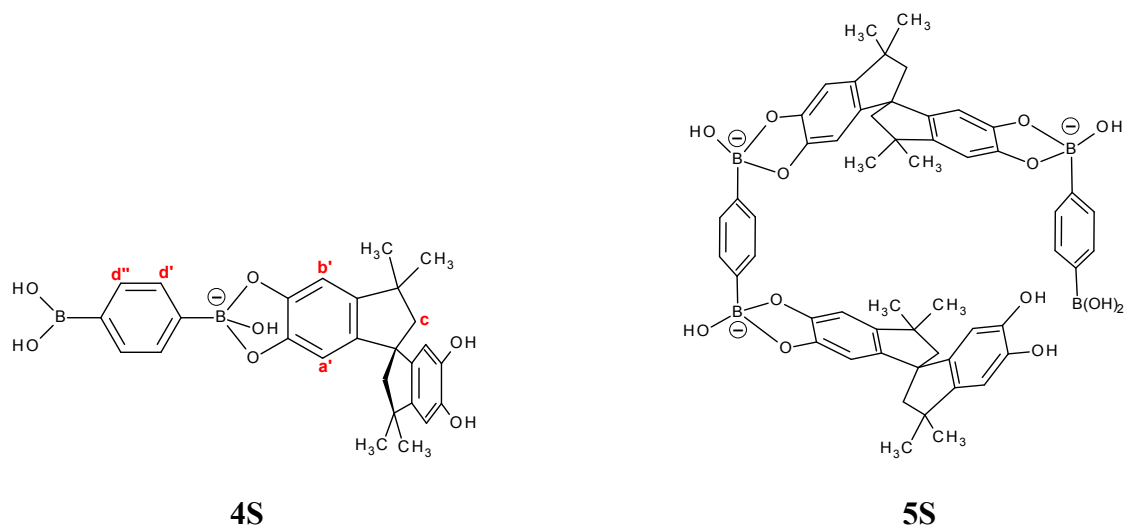


The values of  $p$  and  $q$  ranging from 1 to 3 and values of  $r$  ranging from 1 to 6 were tested in different combinations and the best fit was obtained assuming formation of species  $ASH_{-1}$ ,  $A_2S_2H_{-3}$  and  $A_2S_2H_{-4}$  (note that  $H_{-1}$  in this formalism is equivalent of bound hydroxide anion). The logarithms of equilibrium constants  $\beta_{pqr}$  corresponding to the equation (1) are given in Table 1S.

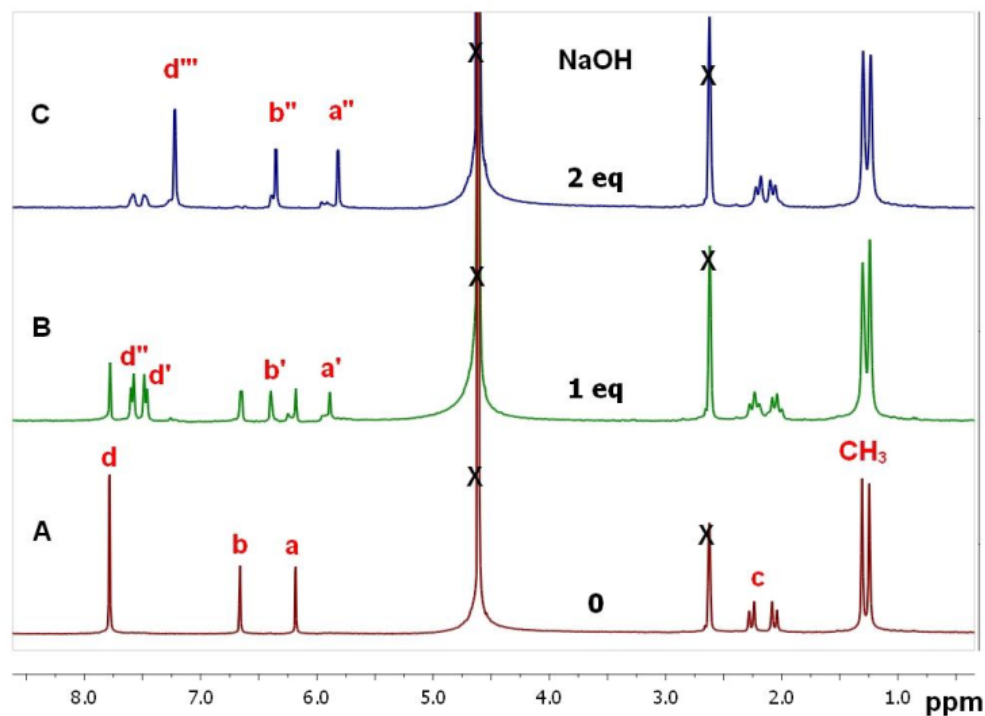
Table 1S. Logarithms of equilibrium constants  $\beta_{pqr}$  corresponding to the equation (1) for dissociation of diboronic acid **2**, dicatechol **1** and formation of boronate esters.

$p$	$q$	$r$	$\log\beta_{pqr}$	reaction
1	0	-1	-10.43±0.05	$R(B(OH)_2)_2 = R(B(OH)_2)(B(OH)_3)^- + H^+$
1	0	-2	-22.91±0.06	$R(B(OH)_2)_2 = R(B(OH)_3)_2^{2-} + 2H^+$
0	1	-1	-10.45±0.03	$R'(OH)_4 = R'(OH)_3(O)^- + H^+$
0	1	-2	-21.87±0.05	$R'(OH)_4 = R'(OH)_2(O)_2^{2-} + 2H^+$
1	1	-1	-5.01±0.02	$R'(OH)_4 + R(B(OH)_2)_2 = (HO)_2R'(O)_2B(OH)R(B(OH)_2)^- + H^+$
2	2	-3	-16.87±0.07	$2R'(OH)_4 + 2R(B(OH)_2)_2 =$ $(HO)_2R'(O)_2B(OH)RB(O)_2(OH)R'(O)_2B(OH)R(B(OH)_2)^{3-} + 3H^+$
2	2	-4	-26.78±0.05	$2R'(OH)_4 + 2R(B(OH)_2)_2 =$ $\overbrace{(O)_2R'(O)_2B(OH)RB(O)_2(OH)R'(O)_2B(OH)R(B(OH))}^{4-} + 4H^+$

The final  $A_2S_2H_{-4}$  complex  $\overbrace{(O)_2R'(O)_2B(OH)RB(O)_2(OH)R'(O)_2B(OH)R(B(OH))}^{4-}$  which is a predominant species in the presence of 2 equivalents of added hydroxide corresponds to **3**. The  $ASH_{-1}$  complex  $(HO)_2R'(O)_2B(OH)R(B(OH)_2)^-$  is a predominant species at  $a=1$  which corresponds to initially formed boronate ester between one catechole group of **1** and one boronic acid group of **2**, structure **4S**. The  $A_2S_2H_{-3}$  complex  $(HO)_2R'(O)_2B(OH)RB(O)_2(OH)R'(O)_2B(OH)R(B(OH)_2)^{3-}$  has its maximum concentration about 40% of total **1** and **2** at  $a=1.5$  and probably has the structure **5S** shown below.



The formation of intermediate complexes was confirmed by  $^1\text{H}$  NMR results. Figure 5S shows  $^1\text{H}$  NMR spectra of a 1:1 mixture of **1** and **2** at increased amounts of added NaOH, which induces formation of tetrahedral anionic boronate ester links.



**Figure 5S.**  $^1\text{H}$  NMR spectra (50% vol.  $\text{DMSO-d}_6/\text{D}_2\text{O}$ ) of the equimolar mixture **1** and **2** (10 mM each) with various equivalents of NaOH. Crossed peaks belong to residual solvent signals.

In the absence of added base (Figure 5SA) one observes a singlet of 4 equivalent phenylene protons of **2** at 7.78 ppm, two singlets of “a” and “b” aromatic protons of **1** and multiplets of methylene and methyl protons of **1**. In the presence of 1 equivalent of NaOH two sets of signals of aromatic protons are clearly seen: one belongs to starting compounds and the other one may be attributed to a 1:1 boronate ester **4S** expected to be the principal product in these conditions. The second set involves a double doublet at 7.5 ppm, which can be attributed to phenylene protons d', d'' in the ester **4S** with non-equivalent boronic acid groups one of which is converted to the boronate ester. There are also two up-field shifted signals of aromatic protons a' and b' which can be attributed to the esterified catechol ring in **4S**. Signals of methyl groups remain unchanged, but methylene signals have increased multiplicity indicating the presence of a mixture of compounds. After addition of the second equivalent of NaOH one observes again a single set of signals with a small proportion of signals at 7.5 ppm which belong to traces of **4S**. The phenylene protons of diboronic acid now give a singlet signal shifted up-field by 0.6 ppm in respect of the signal of free acid. This is in agreement with formation of a bisboronate ester with equivalent anionic boronate groups. Aromatic signals of **1** also are shifted up-field by ca. 0.3 ppm and signals of aliphatic protons remain practically unchanged.

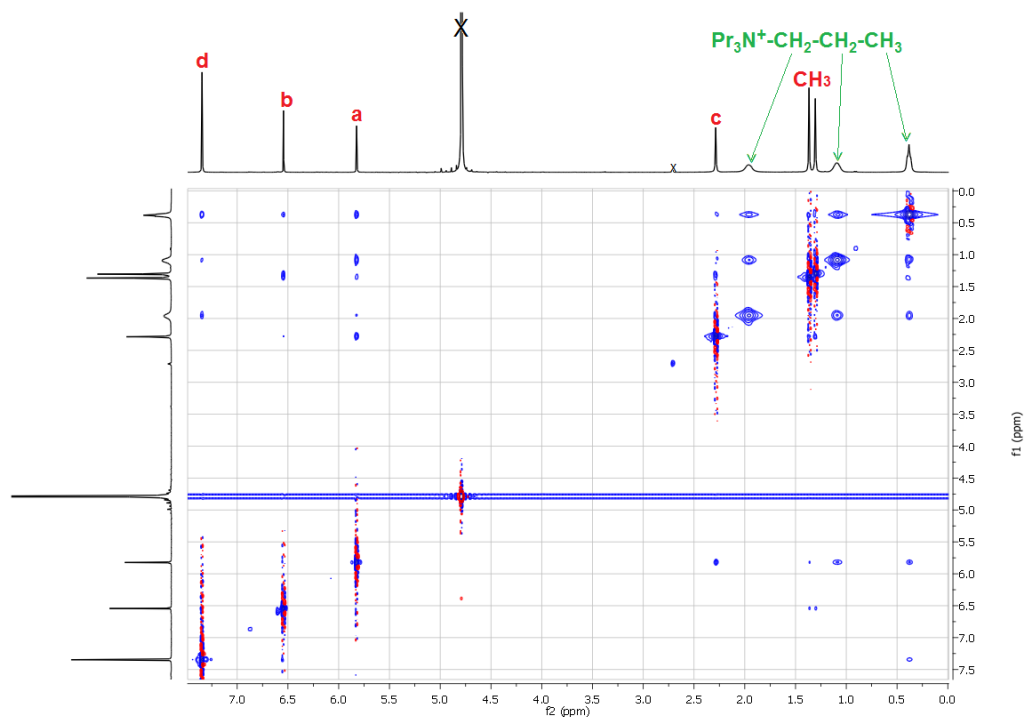


Fig. 6S. NOESY <sup>1</sup>H spectrum of the complex of **3** and  $\text{Pr}_4\text{N}^+$  prepared by mixing 40 mM **1**, 40 mM **2**, 80 mM NaOH and 20 mM  $\text{Pr}_4\text{NCl}$  in 5% vol.  $\text{DMSO-d}_6/\text{D}_2\text{O}$ . Crossed peaks belong to residual solvent signals.

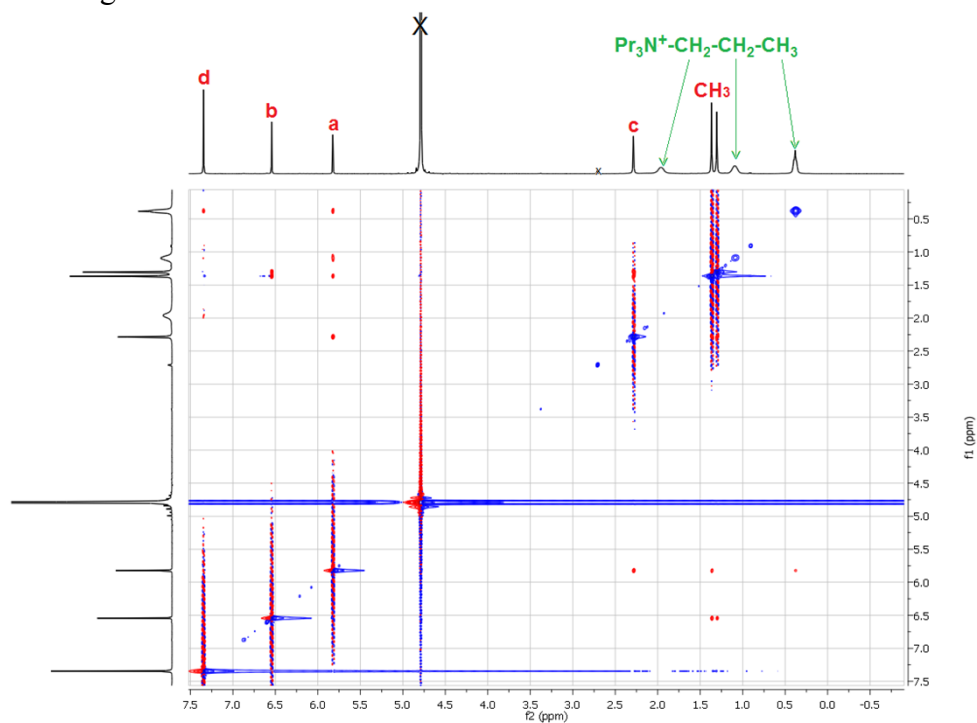


Fig. 7S. ROESY <sup>1</sup>H spectrum of the complex of **3** and  $\text{Pr}_4\text{N}^+$  prepared by mixing 40 mM **1**, 40 mM **2**, 80 mM NaOH and 20 mM  $\text{Pr}_4\text{NCl}$  in 5% vol.  $\text{DMSO-d}_6/\text{D}_2\text{O}$ . Crossed peaks belong to residual solvent signals.

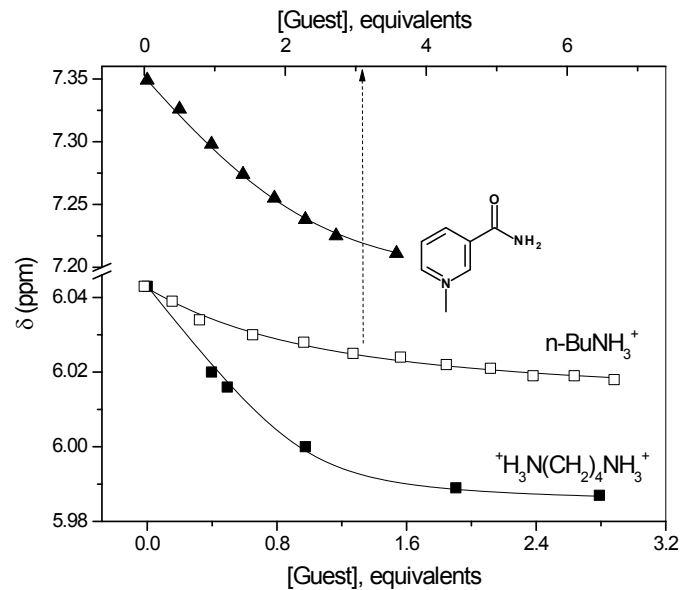


Fig. 8S. Titration plots of 2.5 mM **3** prepared by mixing of 5 mM **1** with 5 mM **2** and 10 mM NaOH in D<sub>2</sub>O containing 5% vol DMSO-d<sub>6</sub> by different cationic guests. The guest concentration is given as number of equivalents to total **3**.



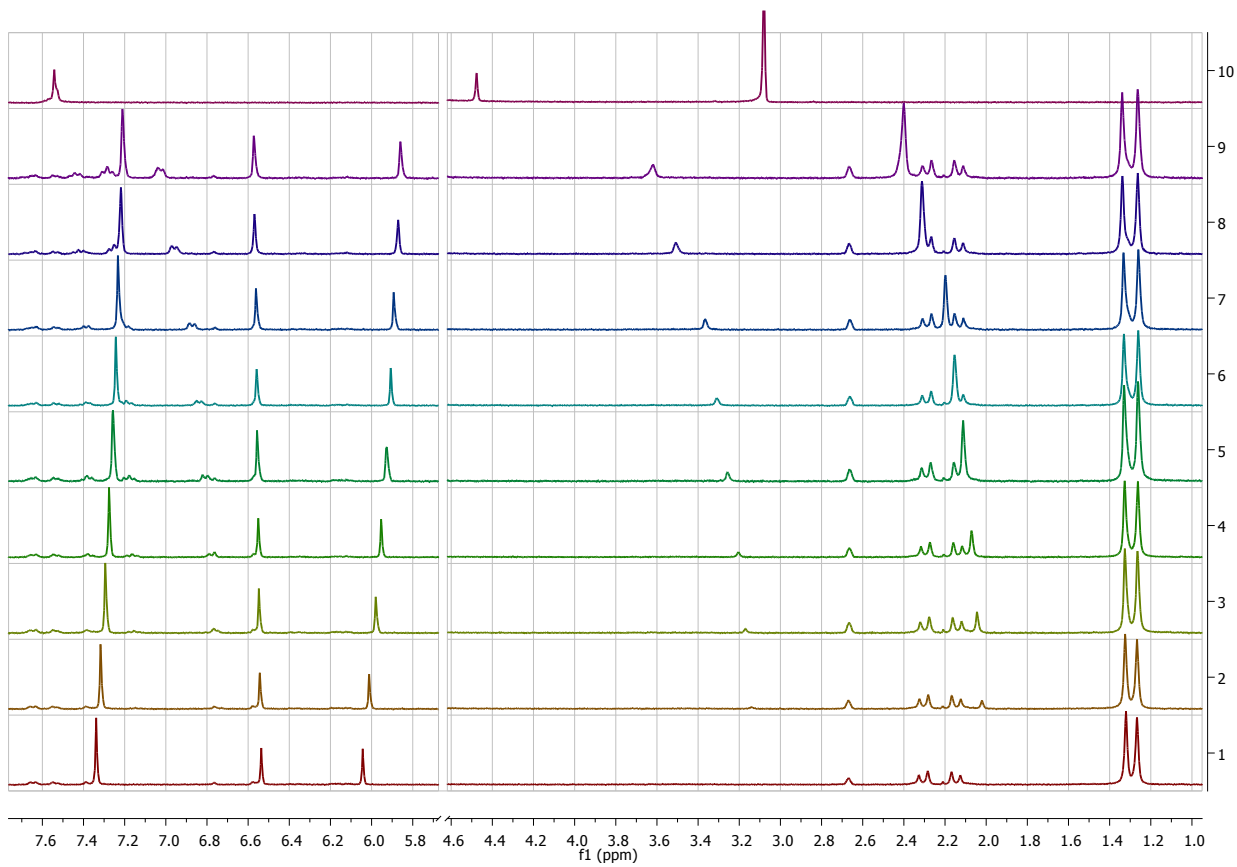


Fig. 9S.  $^1\text{H}$  NMR titration of 2.5 mM **3** by N-benzyltrimethylammonium. Concentrations of N-benzyltrimethylammonium: (1) – 0; (2) – 0.5 mM; (3) - 1.0 mM; (4) – 1.5 mM; (5) – 2.0 mM; (6) – 2.5 mM; (7) – 3.0 mM; (8) – 4.0 mM; (9) – 5.0 mM; (10) – free N-benzyltrimethylammonium.

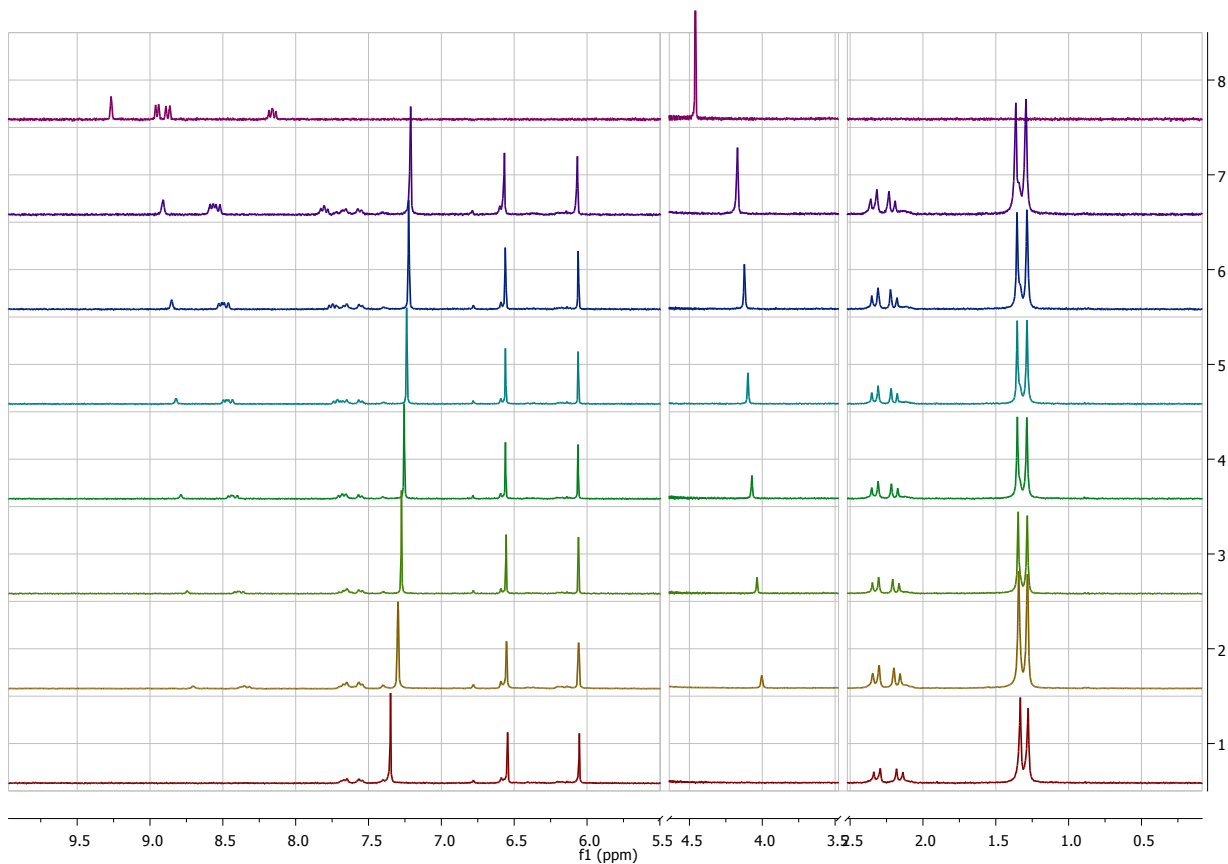


Fig. 10S.  $^1\text{H}$  NMR titration of 2.5 mM **3** by 1-methylnicotinamide. Concentrations of 1-methylnicotinamide: (1) – 0; (2) – 1.0 mM; (3) – 1.5 mM; (4) – 2.0 mM; (5) – 2.5 mM; (6) – 3.0 mM; (7) – 4.0 mM; (8) – free 1-methylnicotinamide.

Table 2S. Computed total energies in au obtained with TeraChem for PBE/6-311++G\*\* method and PBE0/6-311G\*\* method for Berberine

	$\text{Pr}_4\text{N}^+$	$\text{Et}_4\text{N}^+$	$\text{Me}_4\text{N}^+$	Berberine
Free guest	-528.062955	-370.991238	-213.913457	-1127.379119
Free $\text{Na}_4\mathbf{3}$	-3737.689875	-3737.689875	-3737.689875	-3737.644457
Complex	-4265.822007	-4108.752507	-3951.683174	-4865.360458
Interaction	-0.0692	-0.0714	-0.0798	-0.3369

Table 3S. Cartesian coordinates for calculated structures.

Na<sub>4</sub>3

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\*\*\*\*\*

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\*\*\*\*\*

Et<sub>4</sub>N<sup>+</sup>

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