

Short communication

# Extraction and DFT Study on the Complexation of the Sodium Cation with Dibenzo-18-crown-6

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Received: 05-10-2010

## Abstract

From extraction experiments and  $\gamma$ -activity measurements, the extraction constant corresponding to the equilibrium  $\text{Na}^+(\text{aq}) + \text{A}^-(\text{aq}) + \mathbf{1}(\text{nb}) \rightleftharpoons \mathbf{1}\cdot\text{Na}^+(\text{nb}) + \text{A}^-(\text{nb})$  taking place in the two-phase water–nitrobenzene system ( $\text{A}^-$  = picrate,  $\mathbf{1}$  = dibenzo-18-crown-6; aq = aqueous phase, nb = nitrobenzene phase) was evaluated as was  $\log K_{\text{ex}}(\mathbf{1}\cdot\text{Na}^+, \text{A}^-) = 1.7 \pm 0.1$ . Further, the stability constant of the complex  $\mathbf{1}\cdot\text{Na}^+$  in nitrobenzene saturated with water calculated for a temperature of 25 °C:  $\log \beta_{\text{nb}}(\mathbf{1}\cdot\text{Na}^+) = 6.9 \pm 0.1$ . Finally, by using quantum mechanical DFT calculations, the most probable structures of the resulting complex were solved.

**Keywords:** Sodium cation, dibenzo-18-crown-6, complexation, extraction and stability constants, water–nitrobenzene system, DFT, complex structures

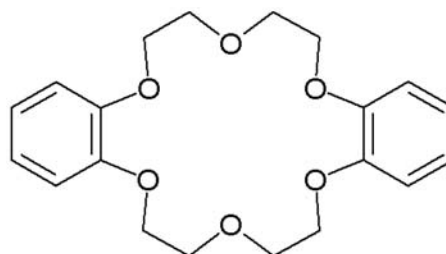
## 1. Introduction

In 1967, Pedersen published his first papers<sup>1,2</sup> dealing with cyclic polyether compounds with oxyethylene groups  $-\text{CH}_2-\text{CH}_2-\text{O}-$ , that are called crowns owing to their structure. These electroneutral compounds form relatively stable complexes in nonaqueous solvents, especially with alkali and alkaline-earth metal cations, the cations being placed in the ligand cavities. The ratio of the size of the crown ligand cavity to the ion radius of the central cation is a decisive or at least an important factor in the stability of the complex compounds formed.<sup>3</sup> It is the complexing properties of the crowns that are due to the rapid development of the chemistry of these cyclic polyethers that we have witnessed in the recent decades. At this point it should be noted that several reviews have covered many aspects of their chemistry.<sup>3–6</sup>

The dicarbollylcobaltate anion<sup>7</sup> and some of its halogen derivatives are very useful reagents for the extraction of various metal cations (especially  $\text{Cs}^+$ ,  $\text{Sr}^{2+}$ ,  $\text{Ba}^{2+}$ ,  $\text{Eu}^{3+}$  and  $\text{Am}^{3+}$ ) from aqueous solutions into a polar orga-

nic phase, both under laboratory conditions for purely theoretical or analytical purposes,<sup>8–29</sup> and on the technological scale for the separation of some high-activity isotopes in the reprocessing of spent nuclear fuel and acidic radioactive waste.<sup>30,31</sup>

In the current work, the stability constant of the cationic complex species  $\mathbf{1}\cdot\text{Na}^+$ , where  $\mathbf{1}$  denotes dibenzo-18-crown-6 (see Scheme 1), in nitrobenzene saturated with water was determined. Moreover, applying quantum mechanical DFT calculations, the most probable structures of the mentioned complex species were predicted.



Scheme 1. Structural formula of dibenzo-18-crown-6 (abbrev.  $\mathbf{1}$ ).

## 2. Experimental

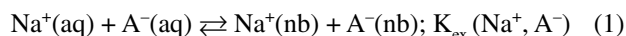
Dibenzo-18-crown-6 (abbrev. **1**; see Scheme 1) was purchased from Fluka. The other chemicals used (Lachema, Brno, Czech Republic) were of reagent grade purity. A solution of sodium picrate (NaA) in water was prepared by dissolving stoichiometric amount of picric acid in an aqueous solution of NaOH. The radionuclide  $^{22}\text{Na}^+$  (DuPont, Belgium) was of standard radiochemical purity.

The extraction experiments were carried out in 10 mL glass test-tubes with polyethylene stoppers: 2 mL of an aqueous solution of NaA of the concentration in the range from  $5 \times 10^{-4}$  to  $1 \times 10^{-3}$  mol/L and microamounts of  $^{22}\text{Na}^+$  were added to 2 mL of a nitrobenzene solution of **1**, the concentration of which varied from  $1 \times 10^{-3}$  to  $2 \times 10^{-3}$  mol/L (in all experiments, the initial concentration of **1** in nitrobenzene,  $C_{\mathbf{1}}^{\text{in,nb}}$ , was always higher than the initial concentration of NaA in water,  $C_{\text{NaA}}^{\text{in,aq}}$ ). The test-tubes filled with the solutions were shaken for 2 h at  $25 \pm 1$  °C, using a laboratory shaker. Then the phases were separated by centrifugation. Afterwards, 1 mL samples were taken from each phase and their  $\gamma$ -activities were measured using a well-type NaI(Tl) scintillation detector connected to a  $\gamma$ -analyzer NK 350 (Gamma, Budapest, Hungary).

The equilibrium distribution ratios of sodium,  $D_{\text{Na}^+}$ , were determined as the ratios of the measured radioactivities of  $^{22}\text{Na}^+$  in the nitrobenzene and aqueous samples.

## 3. Results and Discussion

Regarding the results of previous papers,<sup>7,32</sup> the two-phase water–NaA ( $A^-$  = picrate)–nitrobenzene extraction system can be described by the following equilibrium

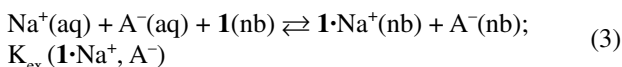


with the corresponding extraction constant  $K_{\text{ex}}(\text{Na}^+, A^-)$ ; aq and nb denote the presence of the species in the aqueous and nitrobenzene phases, respectively. For the constant  $K_{\text{ex}}(\text{Na}^+, A^-)$  one can write<sup>32</sup>

$$\log K_{\text{ex}}(\text{Na}^+, A^-) = \log K_{\text{Na}^+}^i + \log K_{A^-}^i \quad (2)$$

where  $K_{\text{Na}^+}^i$  and  $K_{A^-}^i$  are the individual extraction constants for  $\text{Na}^+$  and  $A^-$ , respectively, in the water–nitrobenzene system.<sup>32</sup> Knowing the values  $\log K_{\text{Na}^+}^i = -6.0$ <sup>32</sup> and  $\log K_{A^-}^i = -0.8$  ( $A^-$  = picrate),<sup>32</sup> the extraction constant  $K_{\text{ex}}(\text{Na}^+, A^-)$  was simply calculated from Eq. (2) as  $\log K_{\text{ex}}(\text{Na}^+, A^-) = -5.2$ .

Previous results<sup>33–37</sup> indicated that the two-phase water–NaA ( $A^-$  = picrate)–nitrobenzene–**1** (**1** = dibenzo-18-crown-6) extraction system, chosen for determination of the stability constant of the complex  $\mathbf{1}\cdot\text{Na}^+$  (see Experimental), can be characterized by the main chemical equilibrium



with the equilibrium extraction constant  $K_{\text{ex}}(\mathbf{1}\cdot\text{Na}^+, A^-)$ :

$$K_{\text{ex}}(\mathbf{1}\cdot\text{Na}^+, A^-) = \frac{[\mathbf{1}\cdot\text{Na}^+]_{\text{nb}}[A^-]_{\text{nb}}}{[\text{Na}^+]_{\text{aq}}[A^-]_{\text{aq}}[\mathbf{1}]_{\text{nb}}} \quad (4)$$

It is necessary to emphasize that **1** is a considerably hydrophobic ligand, practically present in the nitrobenzene phase only, where this ligand forms – with the  $\text{Na}^+$  cation – the relatively stable complex  $\mathbf{1}\cdot\text{Na}^+$ .

Taking into account the conditions of electroneutrality in the organic and aqueous phases

$$[\mathbf{1}\cdot\text{Na}^+]_{\text{nb}} = [A^-]_{\text{nb}} \quad (5)$$

$$[\text{Na}^+]_{\text{aq}} = [A^-]_{\text{aq}} \quad (6)$$

the mass balances of **1** and NaA at equal volumes of the nitrobenzene and aqueous phases

$$[\mathbf{1}\cdot\text{Na}^+]_{\text{nb}} + [\mathbf{1}]_{\text{nb}} = C_{\mathbf{1}}^{\text{in,nb}} \quad (7)$$

$$[\text{Na}^+]_{\text{aq}} + [\mathbf{1}\cdot\text{Na}^+]_{\text{nb}} = C_{\text{NaA}}^{\text{in,aq}} \quad (8)$$

and the measured equilibrium distribution ratio of sodium

$$D_{\text{Na}} = [\mathbf{1}\cdot\text{Na}^+]_{\text{nb}} / [\text{Na}^+]_{\text{aq}} \quad (9)$$

then combination of relationships (4)–(9) gives the final expression for the extraction constant  $K_{\text{ex}}(\mathbf{1}\cdot\text{Na}^+, A^-)$ :

$$K_{\text{ex}}(\mathbf{1}\cdot\text{Na}^+, A^-) = D_{\text{Na}}^2 / \left\{ C_{\mathbf{1}}^{\text{in,nb}} - \frac{D_{\text{Na}}}{1 + D_{\text{Na}}} C_{\text{NaA}}^{\text{in,aq}} \right\} \quad (10)$$

In this study, from the extraction experiments and  $\gamma$ -activity measurements (see Experimental) by means of Eq. (10), the following value of the constant  $K_{\text{ex}}(\mathbf{1}\cdot\text{Na}^+, A^-)$  was determined:  $\log K_{\text{ex}}(\mathbf{1}\cdot\text{Na}^+, A^-) = 1.7 \pm 0.1$ .

Furthermore, with respect to previous results,<sup>33–37</sup> for the extraction constants  $K_{\text{ex}}(\text{Na}^+, A^-)$  and  $K_{\text{ex}}(\mathbf{1}\cdot\text{Na}^+, A^-)$  defined above, as well as for the stability constant of the complex  $\mathbf{1}\cdot\text{Na}^+$  in nitrobenzene saturated with water, denoted by  $\beta_{\text{nb}}(\mathbf{1}\cdot\text{Na}^+)$ , one gets

$$\log \beta_{\text{nb}}(\mathbf{1}\cdot\text{Na}^+) = \log K_{\text{ex}}(\mathbf{1}\cdot\text{Na}^+, A^-) - \log K_{\text{ex}}(\text{Na}^+, A^-) \quad (11)$$

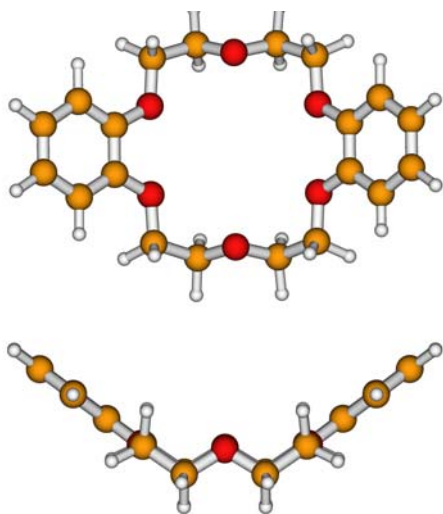
Using the constants  $\log K_{\text{ex}}(\text{Na}^+, A^-)$  and  $\log K_{\text{ex}}(\mathbf{1}\cdot\text{Na}^+, A^-)$  given above, and applying Eq. (11), we obtain the stability constant of the  $\mathbf{1}\cdot\text{Na}^+$  complex in water-saturated nitrobenzene at 25 °C as  $\log \beta_{\text{nb}}(\mathbf{1}\cdot\text{Na}^+) = 6.9 \pm 0.1$ , which is in relatively good agreement with the value  $\log \beta_{\text{nb}}(\mathbf{1}\cdot\text{Na}^+) = 7.1$  (**1** = dibenzo-18-crown-6) determined previously.<sup>33</sup>

The quantum mechanical calculations were carried out at the density functional level of theory (DFT, B3LYP functional) using the Gaussian 03 suite of programs.<sup>38</sup> The 6-31G(d) basis set was used and the optimizations were unconstrained. Although a possible influence of a polar solvent on the detailed structures of **1** and the complex species with Na<sup>+</sup> could be imagined, our quantum mechanical calculations in similar cases, performed in an analogous way, showed very good agreement of experiment with theory.<sup>39–44</sup>

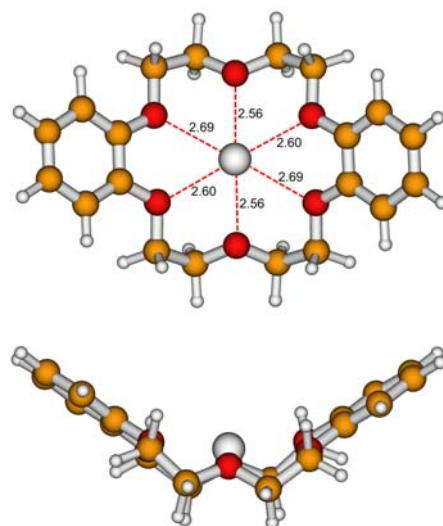
Iwachido et al.<sup>45</sup> determined the hydration number of the dibenzo-18-crown-6·Na<sup>+</sup> (i. e., **1**·Na<sup>+</sup>) complex in the organic phase of the water–nitrobenzene extraction system as  $h(\mathbf{1}\cdot\text{Na}^+) = 1.2$ . Thus, in our study, let us consider further both the “nonhydrated” state (**1**·Na<sup>+</sup>) and the “hydrated” state (**1**·Na<sup>+</sup>·H<sub>2</sub>O) of the mentioned complex species.

In the model calculations, we optimized the molecular geometries of the parent dibenzo-18-crown-6 ligand **1** and its cationic complex species with Na<sup>+</sup>. The optimized structure of a free ligand **1** with C<sub>2</sub> symmetry is illustrated in Figure 1. In Figure 2, the most energetically favoured structure obtained by the DFT optimization of the **1**·Na<sup>+</sup> complex having also C<sub>2</sub> symmetry is depicted, together with the lengths of the corresponding strong Na<sup>+</sup>···O bonds (in Å; 1 Å = 0.1 nm). The calculated binding energy of this complex is 376.5 kJ/mol.

The structures A and B obtained by the full DFT optimizations of the cationic complex species **1**·Na<sup>+</sup>·H<sub>2</sub>O are shown in Figures 3 and 4, respectively, including the lengths of the corresponding strong bonds. Besides, it should be noted that the structure B of the considered “hydrated” complex **1**·Na<sup>+</sup>·H<sub>2</sub>O is stabilized by strong hydrogen bond OH···O (2.03 Å) as well. The binding energies corresponding to the structures A and B were found to be very close: 450.4 and 449.7 kJ/mol, respectively.

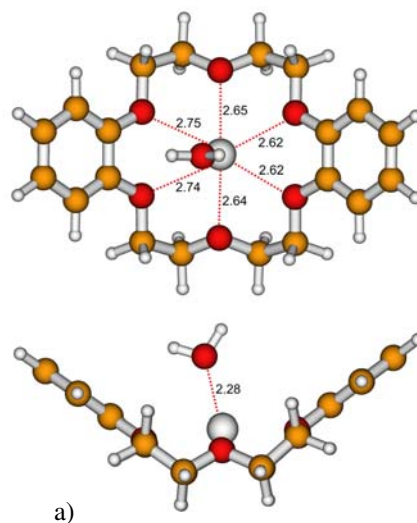


**Figure 1.** Two projections of the DFT optimized structure of a free ligand **1** [B3LYP/6-31G(d)].



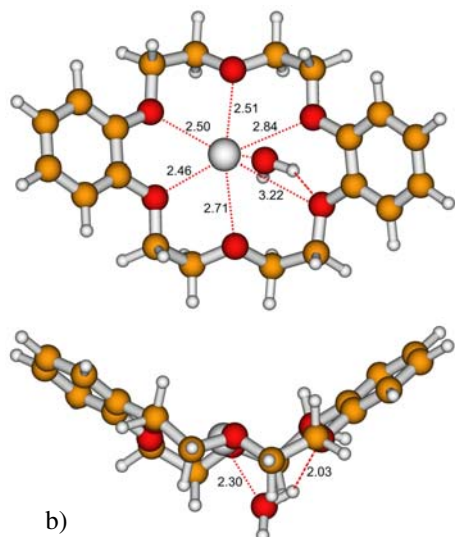
**Figure 2.** Two projections of the DFT optimized structure of the **1**·Na<sup>+</sup> complex [B3LYP/6-31G(d)]. The Na<sup>+</sup>···O distances: 2.69, 2.56, 2.60, 2.69, 2.60, and 2.56 Å.

vely. From these data it follows that the structures A and B of the resulting complex **1**·Na<sup>+</sup>·H<sub>2</sub>O are apparently in a dynamic equilibrium.



**Figure 3.** Two projections of the DFT optimized structure A of the **1**·Na<sup>+</sup>·H<sub>2</sub>O complex [B3LYP/6-31G(d)]. The Na<sup>+</sup>···O (of the parent ligand **1**) distances: 2.74, 2.75, 2.65, 2.62, 2.62, and 2.64 Å; the Na<sup>+</sup>···O (of the water molecule) distance: 2.28 Å.

In conclusion, it is necessary to emphasize that the optimized structures A and B of the **1**·Na<sup>+</sup>·H<sub>2</sub>O cationic complex species (see Figures 3 and 4) are evidently much more real than that of the complex **1**·Na<sup>+</sup> presented in Figure 2. This fact is confirmed especially by the respective binding energies given above.



**Figure 4.** Two projections of the DFT optimized structure B of the  $1 \cdot \text{Na}^+ \cdot \text{H}_2\text{O}$  complex [B3LYP/6-31G(d)]. The  $\text{Na}^+ \cdots \text{O}$  (of the parent ligand 1) distances: 2.46, 2.50, 2.51, 2.84, 3.22, and 2.71 Å; the  $\text{Na}^+ \cdots \text{O}$  (of the water molecule) distance: 2.30 Å; the hydrogen bond  $\text{OH} \cdots \text{O}$  length: 2.03 Å.

## 4. Acknowledgements

This work was supported by the Czech Ministry of Education, Youth and Sports (Projects MSM 4977751303 and MSM 6046137301) and by the Czech Science Foundation (Project P205/10/2280). The computer time at the MetaCentrum (Project MSM 6383917201), as well as at the Institute of Physics (computer Luna/Apollo), Academy of Sciences of the Czech Republic, is gratefully acknowledged.

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## Povzetek

V dvofaznem sistemu voda-nitrobenzen smo proučevali ravnotežje  $\text{Na}^+(\text{aq}) + \text{A}^-(\text{aq}) + \mathbf{1}(\text{nb}) \rightleftharpoons \mathbf{1}\cdot\text{Na}^+(\text{nb}) + \text{A}^-(\text{nb})$ ,  $\text{A}^-$  = pikrat,  $\mathbf{1}$  = dibenzo-18-crown-6; aq = vodna faza, nb = nitrobenzen). Z meritvami množine porazdelitve posameznih snovi med obe fazi smo določili konstanto ekstrakcije,  $\log K_{\text{ex}}(\mathbf{1}\cdot\text{Na}^+, \text{A}^-) = 1.7 \pm 0.1$ . Določili smo tudi konstanto stabilnosti kompleksa pri 15 °C  $\mathbf{1}\cdot\text{Na}^+$  v nitrobenzenu, nasičenem z vodo,  $\log \beta_{\text{nb}}(\mathbf{1}\cdot\text{Na}^+) = 6.9 \pm 0.1$ . S kvantno mehanskimi DFT računi smo predvideli tudi najbolj verjetno strukturo tega kompleksa.