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Recognition of steric factor in external association of xanthenocrown-5 and *bis*-napthalenocrown-6 with bis(benzimidazolium)propane borontetrafluoride

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ABSTRACT

This is the first report of charge transfer band for crown-axel H-bonding interaction in acetonitrile medium. Monte Carlo simulation established external association of small cavity crown with BBIM-propane dication axels. Resonance energy, binding constant and ratiometric detection of association of xanthenocrown-5 (**1**) and *bis*-napthalenocrown-6 (**2**) with *bis*-(benzimidazolium)propane borontetrafluoride (**3a–3d**) in acetonitrile determined the effect of steric factor towards association.

1. Introduction

The association of one molecule with another deals with the possibility of H-bonding, π–π interaction, v.d.W. forces and hydrophobic interactions [1]. The extent of interaction depends on many factors including electron donating/accepting property of molecules [2], steric factor [3], solvent environment [4] and orientation of the interacting templates [5]. Supramolecular rotaxane, pseudorotaxane formation or external association in crown-axel type interacting system depends on the cavity size of crown [6], size, shape and charge of axel [7], catalytic factor [8], and orientation of axel-crown pair along with steric congestion.

In the present study, two sterically hindered crown ethers viz. xanthenocrown-5 (**1**) and *bis*-napthalenocrown-6 (**2**) (Fig. 1) were synthesized from 2-naphthol (Schemes 1 and 2). External association is expected with such small cavity crown ethers on interacting with *bis*-(benzimidazolium)propane borontetrafluoride (BBIM-propane, **3a-d**) axels (Fig.1) in acetonitrile as threading is not possible [9]. Crown **1** is like a yatch, in which xanthene group is a fixed sail while crown **2** contains two naphthalene rings connected to a tetrahedral carbon with a phenyl ring. Interaction of four different BBIM-propanes with these two crown ethers have been studied photophysically. Clear CT bands were observed in the UV region for all the eight interacting systems. Both the crown ethers exhibited most feasible interaction with least crowded axel (**3a**) in acetonitrile. However, the axel **3a**, demonstrated the highest binding adduct with the less sterically hindered crown **2** both in the ground as well as in the excited states. Thus, steric factor is recognized with highest stability of adduct **2**/**3a** even when external association is taking place in crown–axel interaction. Monte Carlo simulation study further substantiated the experimental data.

2. Experimental

2.1. Materials and methods

HPLC grade acetonitrile used as solvent in all the experiments. Four *bis*-(benzimidazolium)propane borontetrafluoride compounds were prepared following the reported procedure [10]. The two crown ethers used in this study are Xanthenocrown-5 (**1**) and *bis*-Napthalenocrown-6 (**2**) among which crown **2** is already reported [11], but the sterically hindered crown **1** is newly synthesized. Both are reported here.

2.2. Instruments used

The absorption (UV–vis) spectral measurements were performed with a Shimadzu UV 1800 spectrophotometer fitted with an electronic

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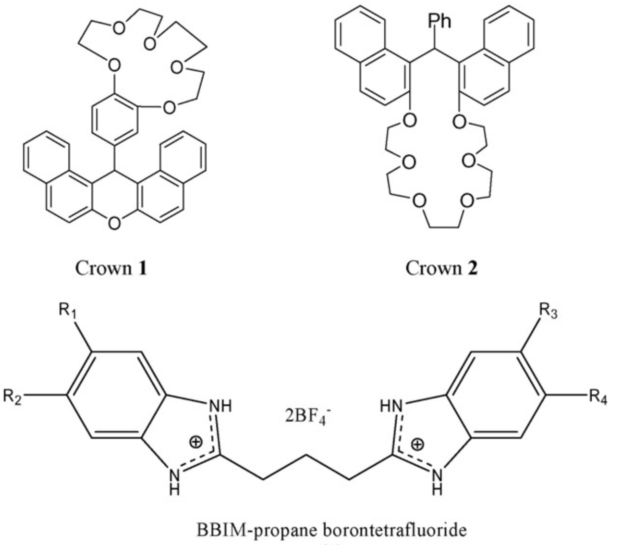


Crown **1** Crown **2**

BBIM-propane borontetrafluoride
(**3**)

(**3a**) $R_1 = R_2 = R_3 = R_4 = H$;
(**3b**) $R_1 = R_2 = CH_3$, $R_3 = R_4 = H$;
(**3c**) $R_1 = R_3 = CH_3$, $R_2 = R_4 = H$;
(**3d**) $R_1 = R_2 = R_3 = R_4 = CH_3$.

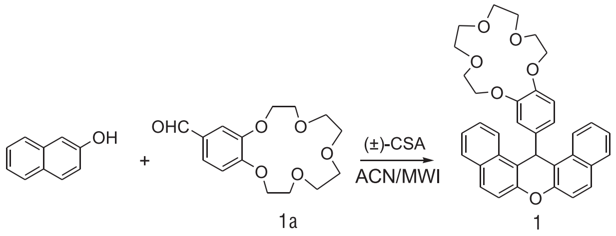
Fig. 1. Structure of the xanthenocrown-5 (**1**) and *bis*-napthalenocrown-6 (**2**) and bis(benzimidazolium)propane borontetrafluoride (BBIM-propane axels) (**3a**–**3d**).

temperature controller unit (TCC — 240 A). The steady state fluorescence emission and excitation spectra were recorded with a Hitachi F-4500 spectrofluorometer equipped with a temperature controlled cell holder. Temperature was controlled within ±0.1 K by circulating water from a constant temperature bath (Heto Holten, Denmark). Monte Carlo simulations were performed using Spartan'14 molecular modeling software from Wavefuntion Inc. (Irvine, CA, USA). Using Monte Carlo simulation [12], global minima search for all the eight optimized complexes neglecting solvent were performed using Merck molecular force-field calculations (MMFF). Energy of the simulated equilibrium conformers as well as global minima were calculated using single point calculation by DFT/MPW1PW91 functional using 6-31G* basis set in Gaussian09.

2.3. Synthetic procedure of crown 1 and crown 2

Xanthenocrown-5 (**1**): A mixture of 2-naphthol (1.44 g, 10 mmol), 4-formyl benzo-15-crown-5 (**1a**) (1.63 g, 5.5 mmol) and (±)-camphor-10-sulfonic acid (CSA) (0.17 g, 0.75 mmol) in 2 ml of acetonitrile was taken in a microwave vessel and irradiated (400 W, 63–64 °C) under microwave. After 45 min, TLC showed complete consumption of the starting material (2-naphthol) and formation of **1** as the only product. The reaction mixture was quenched with saturated aqueous sodium bicarbonate solution and extracted with ethyl acetate. The organic layer was washed with brine, dried (Na_2SO_4) and evaporated under reduced pressure to obtain a thick mass which was purified by column chromatography on silica using $CHCl_3$ as eluant to afford pure **1** (2.52 g, 92%).

1: pink solid; mp 187–188 °C; IR ($CHCl_3$): υ 3017, 2929, 1636, 1593, 1513, 1456, 1431, 1401, 1250, 1240, 1215, 1139 cm^{-1}; ^{1}HNMR (200 MHz, $CDCl_3$): δ 3.62 (s, 8 H, 4 × OCH_2CH_2O), 3.72–3.80 (m, 4 H, 2 × OCH_2CH_2O), 3.91–3.93 (m, 4 H, 2 × OCH_2CH_2O), 6.41 (s, 1 H, ArCHAr), 6.63 (d, $J = 8.2$ Hz, 1 H, ArH), 6.93–6.94 (m, 1 H, ArH), 7.08 (dd, $J = 8.2, 1.8$ Hz, 1 H, ArH),7.37–7.48 (m, 4 H, ArH), 7.53–7.60 (m, 2 H, ArH), 7.80 (t, $J = 9.1$ Hz, 4 H, ArH), 8.37 (d, $J = 8.5$ Hz, 2 H, ArH); ^{13}C NMR (50 MHz, $CDCl_3$): δ 37.3, 69.0, 69.1, 69.5, 70.6, 70.9, 114.0, 114.9, 117.4, 117.8, 121.1, 122.7, 124.1, 126.6, 128.7, 131.0, 131.4138.2, 147.7, 148.7, 149.1; MS, m/z (%) = 571 (M^+Na, 100).



Scheme 1. Synthetic scheme of crown 1.

1,1-*bis*-(2-hydroxynaphthyl)phenylmethane (**2a**): A mixture of 2-naphthol (1.44 g, 10 mmol), benzaldehyde (0.584 g, 5.5 mmol) and (±)-camphor-10-sulfonic acid (0.232 g, 1.0 mmol) in dry acetonitrile was stirred at ambient temperature (25 °C). After 16 h, TLC showed complete consumption of both the starting materials. The solid thus formed was quenched with water, filtered, washed with water and dried in air. The crude solid was recrystallized with hexane-ethyl acetate to afford pure **2a** (1.41 g, 75%).

2a: pink solid; mp 195–196 °C; IR ($CHCl_3$): υ 3471, 3423, 3019, 1618, 1597,1513, 1491, 1468, 1390, 1253, 1046, 877 cm^{-1}; ^{1}H NMR (200 MHz, CD_3COCD_3): δ 7.13–7.38 (m, 12 H, ArCHAr, ArH), 7.74–7.84 (m, 4 H, ArH), 8.12 (d, $J = 8.3$ Hz, 2 H, ArH); ^{13}C NMR (50 MHz, CD_3COCD_3): δ 43.0, 120.1, 120.4, 123.6, 123.7, 126.8, 127.5, 128.8, 129.1, 129.7, 130.0, 130.5, 135.2, 143.3, 154.0; HRMS: m/z calc. for $C_{27}H_{20}O_2Na$ (M^+Na): 399.1361; found: 399.1365.

***bis*-Napthalenocrown-6** (**2**): A mixture of **2a** (0.790 g, 2.1 mmol), pentaethyleneglycolditosylate (1.26 g, 2.3 mmol, 1.1 equiv) and Cs_2CO_3 (1.73 g, 5.3 mmol, 2.5 equiv) in dry acetonitrile (30 ml) was refluxed for 8 h when TLC showed complete consumption of both **2a** and the ditosylate. The solvent was removed under *vacuo*, cooled, quenched with 1 N HCl and extracted with ethyl acetate. The organic layer was washed with water, brine and dried (Na_2SO_4). Removal of solvent afforded a thick mass which was purified by silica gel column chromatography (using $CHCl_3$ as eluant) to afford pure **2** (0.948 g, 78%).

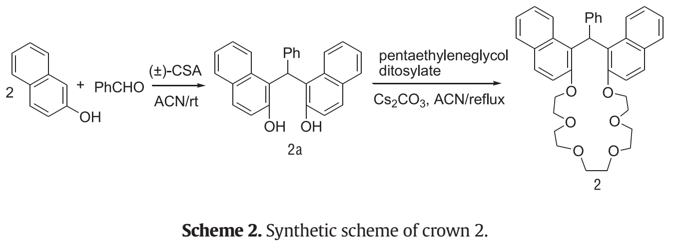
2: light yellow solid; mp 155–156 °C; IR ($CHCl_3$): υ 3058, 3016, 2874, 1622, 1598, 1511, 1492, 1451, 1451, 1295, 1259, 1243,1215, 1176, 928, 806, 697 cm^{-1}; ^{1}H NMR (200 MHz, $CDCl_3$): δ 2.88–2.98 (m, 2 H, OCH_2CH_2O), 3.10–3.21 (m, 2 H, OCH_2CH_2O),3.31–3.35 (m, 4 H, 2 × OCH_2CH_2O), 3.45–3.48 (m, 8 H, 4 × OCH_2CH_2O), 3.69–3.71 (m, 2 H, OCH_2CH_2O), 3.77–3.83 (m, 2 H,OCH_2CH_2O), 7.03–7.14 (m, 6 H, ArCHAr, ArH), 7.23–7.30 (m, 6 H, ArH), 7.73–7.81 (m, 6 H, ArH); ^{13}C NMR (50 MHz, $CDCl_3$):

δ 43.9, 68.4, 68.9, 70.3, 116.1, 122.7124.0, 124.8, 125.2, 125.8, 127.5, 128.1, 128.2, 128.7, 129.4, 133.4, 144.9, 155.2; HRMS:m/z calc. for $C_{37}H_{39}O_6$ (M^+H): 579.2747; found: 579.2731.

3. Result and discussions

3.1. Photophysical study

Fig. 2 shows the electronic absorption spectra of two mixtures containing (**1** + **3d**) and (**2** + **3d**) respectively in acetonitrile medium. To obtain the CT bands, spectra of above solution (in acetonitrile medium)



Scheme 2. Synthetic scheme of crown 2.

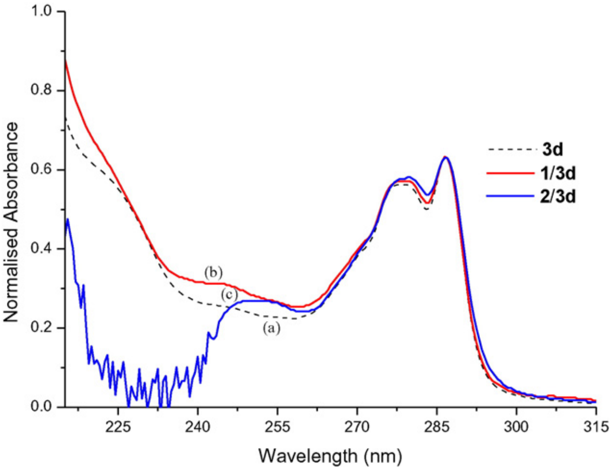


Fig. 2. (a) Absorption spectra of **3d** plotted along with the solvent as reference. Charge transfer absorption spectra of (b) **1** (5.46×10^{-5} mol·dm^{-3}) + **3d** (6.26×10^{-6} mol·dm^{-3}); (c) **2** (5.18×10^{-5} mol·dm^{-3}) + **3d** (6.26×10^{-6} mol·dm^{-3}) mixtures plotted along with the pristine donor solution as reference.

Table 1
CT absorption maxima and transition energies for the complexes of **1** and **2** with **3a**, **3b**, **3c** and **3d** in acetonitrile.

System	λ_{CT} (nm)	$h\nu_{CT}$ (eV)	f (dm^3·mol^{-1}·cm^{-2})	μ_{EN} (Debye)	$\|R_N\|$ (eV)
1/3a	246.4	5.027	0.3623	10.13	0.41803
1/3b	239.2	5.18	0.02096	5.13	0.14103
1/3c	237.6	5.22	0.0467	5.57	0.1645
1/3d	239.9	5.17	0.0567	6.23	0.1987
2/3a	251.3	4.935	0.214	11.93	0.5118
2/3b	249.1	4.979	0.01185	4.28	0.0949
2/3c	252.1	4.92	0.2408	11.62	0.4929
2/3d	251.0	4.941	0.02404	5.21	0.1385

were recorded against the pristine crown ether solution as reference to cancel out the donor absorbance. It was observed that new absorption peaks appear in the UV region.

Similar spectral features have been obtained with mixtures containing (**1** + **3a**), (**1** + **3b**), (**1** + **3c**) and (**2** + **3a**), (**2** + **3b**), (**2** + **3c**) also. The CT absorption spectra were characterized by fitting to the usual Gaussian function [13]. A representative plot was shown in Fig. 3. The results of the Gaussian analysis for all the **1**-axel and **2**-axel systems under study were shown in Table 1. The wavelengths at these new absorption maxima ($\lambda_{max} = x_c$) and the corresponding transition energies ($h\nu$) are summarized in Table 1. The Gaussian analysis fitting was done using the method developed by Gould et al. [14]. The observed oscillator strengths of the CT bands are summarized in Table 1 for all the eight complexes. Values of μ_{EN} for the complexes of both **1** and **2** with four different electron acceptors are given in Table 1. The oscillator strength (f) is proportional to the square of transition dipole $|\mu_{EN}|^2$. The higher observed oscillator strength for the **1**/**3a**, **2**/**3a** and **2**/**3c** complexes in acetonitrile as recorded in Table 1 might reflect the higher transition dipole when there is enough scope for the formation of stable π–π stacking and H-bonding interaction of crowns **1** and **2** with axels **3a** and **3c** respectively. In case of **3a** possibility of both π–π stacking and H-bonding interaction prevails for both crowns **1** and **2**. R_N is the resonance energy of the complex in the ground state, which, obviously is a contributing factor to the stability constant of the complex (a ground state property). The values of R_N for the complexes under study have also been given in Table 1. Trend in R_N value shows that **3a** forms the most stable complex with both **1** and **2** compared to other axels. **3c** also forms a strong complex with **2**. On contrary, exceptionally poor stability were found with **3b** adducts in case of both the crowns.

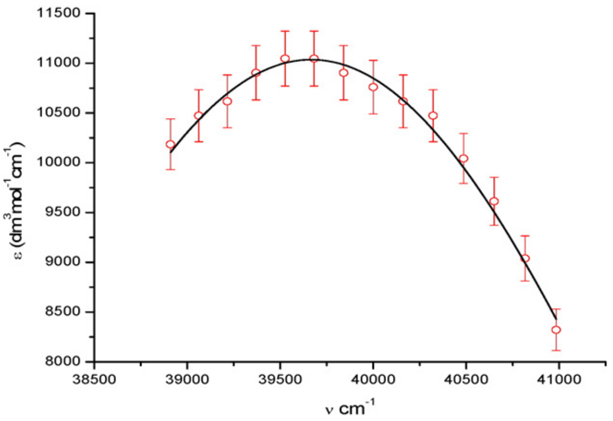


Fig. 3. Gaussian curve analysis of the shoulder region of the CT band for **2**/**3c** system in acetonitrile.

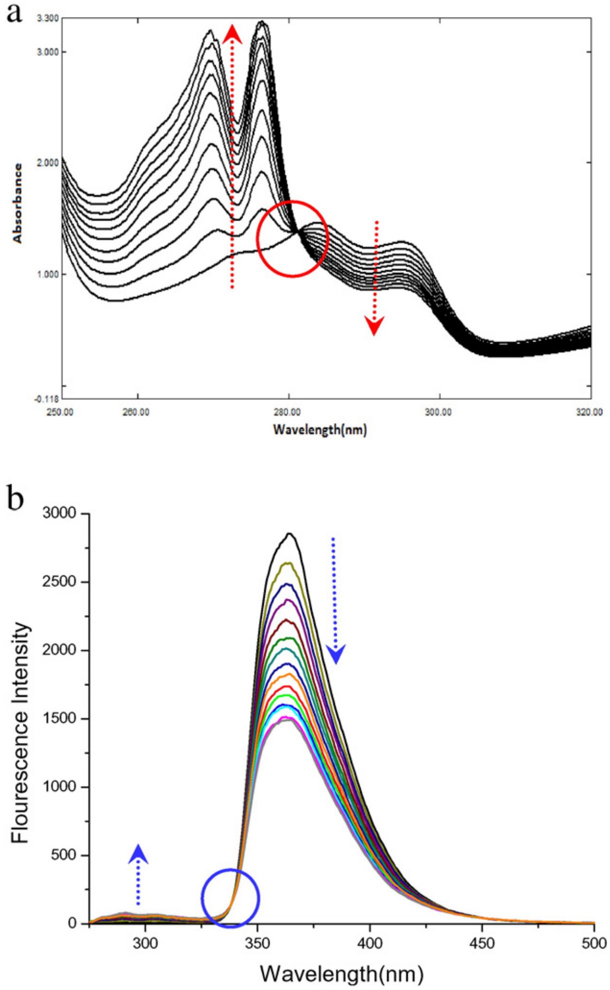


Fig. 4. [a] Ground state isosbestic formation between crown **2** and the axel **3a** in acetonitrile medium. Concentration of axel **3a**: 0.00, 1.724×10^{-5}, 3.29×10^{-5}, 4.72×10^{-5}, 6.03×10^{-5}, 7.24×10^{-5}, 8.35×10^{-5}, 9.38×10^{-5}, 1.03×10^{-4}, 1.123×10^{-4} and 1.21×10^{-4} M·dm^{-3} at a fixed concentration of crown **2** (1.227×10^{-4} mol·dm^{-3}) in acetonitrile. [b] Excited state titration of the crown **2** by axel **3a** in acetonitrile. Concentration of axel **3a**: 0.00, 5.07×10^{-6}, 9.68×10^{-6}, 1.39×10^{-5}, 1.775×10^{-5}, 2.13×10^{-5}, 2.45×10^{-5}, 2.76×10^{-5}, 3.04×10^{-5}, 3.3×10^{-5} and 3.55×10^{-5}, 3.78×10^{-5}, 3.99×10^{-5}, 4.19×10^{-5} and 4.38×10^{-5} M·dm^{-3} at a fixed concentration of crown **2** (1.227×10^{-4} mol·dm^{-3}) in acetonitrile. $\lambda_{ex} = 300$ nm.

Table 2
Isosbestic points appeared on interaction of axel **3a** with the two crown ethers (**1** and **2**) along with their ground and excited state association constant values in acetonitrile.

System	Absorption isosbestic points at wavelength (nm)	Iso-emissive points at wavelength (nm)	Association constant (M^{-1})	
			Ground state ($K_{BH} \times 10^{-4}$)	Excited state ($K_{SV} \times 10^{-3}$)
1/**3a**	281.24	337.2, 398.6	8.71	6.49
2/**3a**	295.00	338.0	147.80	13.90

Thus, CT interaction parameters clearly indicate that **3a** forms most stable adducts with both the crown ethers (**1** and **2**) in acetonitrile. But **3c** having a methyl substitution in both the benzimidazole rings on BBIM-propane unit, can establish equally stable adduct in the ground state with crown **2** only, but not with **1**. This might be because of heavy steric congestion that prevails in the xanthene unit of crown **1**.

To find out the details on the type of interaction that took place between **3a** and the two crowns (**1** and **2**), titration of fixed concentration crown solution with the axel **3a** in acetonitrile was attempted seperately. Both the crowns (**1** and **2**) have demonstrated well established isosbestic points (Fig. 4(a)) in the absorption study as well as iso-emissive points (Fig 4(b)) in the fluorescence study (in Table 2). Thus, **3a** forms well defined equilibrium with both **1** and **2** in the ground as well as in the excited state.

In our previous work, BBIM-propane salts threaded the cavity of DB24C8 [15] and not less [9]. Threading of BBIM-propane salts failed with the next higher available crown DB30C10 [16]. Consequently, here with the two crown ethers (**1** is crown-5 and **2** is crown-6) have lower cavity size than that of crown-8, external association is expected as was observed in case of other crown-5 [9].

Association constant both in ground as well as in excited state (shown in Table 2) indicated the extent of association of axel **3a** with the two crown ethers in acetonitrile medium. Ground state Benesi–Hildebrand [17] association constant (K_{BH}) for 1:1 adduct and the excited state Stern–Volmer [18] constant (K_{SV}) follows the same order, **1** ≪ **2**, as was observed analyzing the CT parameters discussed above. Fig. 5 shows the collective BH and SV plots of the two crown ethers for **3a** axel.

3.2. Monte Carlo simulation

A rigorous Monte Carlo conformational search protocol [12] was employed for better understanding of these associated complexes. Using Monte Carlo simulation, equilibrium conformer searching over 2500 possible conformers for all the eight complexes neglecting anion and solvent were performed using Merck molecular force-field calculations (MMFF). Fig. 6 represented two such global minimum conformers. Crown **1** with all the four axels (**3a**–**d**) form a similar type of global minimum conformers where only one H-bond of O—H bond distance (1.7–1.8) Å is formed with the O-3, the terminal oxygen far from steric congestion of xanthene ring. However, for **2**, all four axels form two H-bonds along with the possibility of π–π stacking in external association (shown in Table 3). This stronger H-bond formation along with

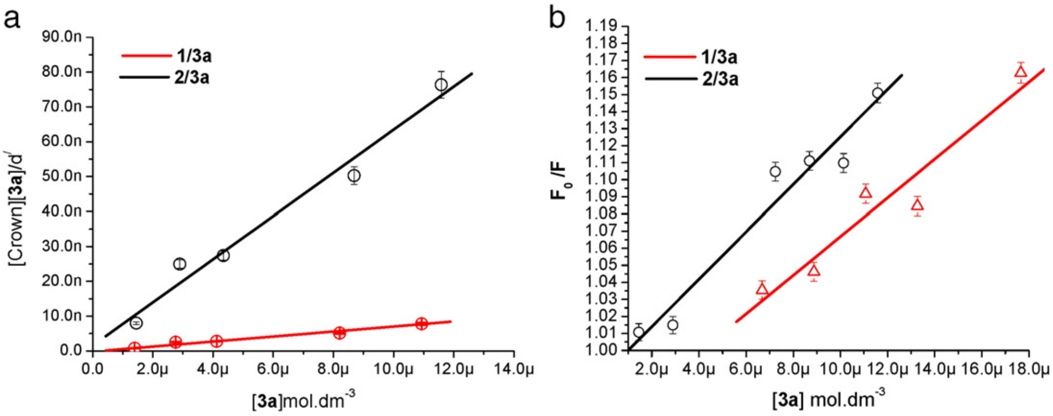
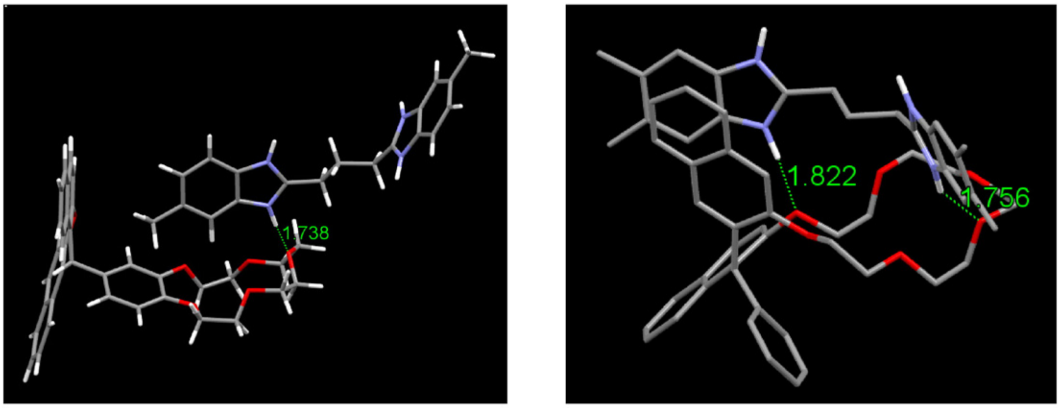


Fig. 5. (a) Benesi–Hildebrand and (b) Stern–Volmer binding constant of two crown ethers **1** and **2** with axel **3a** in acetonitrile.



(A) (B)

Fig. 6. The global minimum conformer of the adducts (A) **1**/**3c** and (B) **2**/**3d** obtained in Monte Carlo simulation. All hydrogen atoms except those involved in H-bonding are removed for clarity in the last perspective.

Table 3
Parameters of Monte Carlo global minimum conformers in crown-axel adducts.

System	H-bond distance (Å)	Angle between benzimidazole ring and crown aromatic ring (°)
1/**3a**	1.757	86.47
1/**3b**	1.742	84.59
1/**3c**	1.738	82.35
1/**3d**	1.830	58.62
2/**3a**	1.652, 1.653	11.05
2/**3b**	1.758, 1.823	17.05
2/**3c**	1.742, 1.792	9.71
2/**3d**	1.756, 1.822	17.21

π–π stacking of benzimidazole ring and the crown naphthalene ring might be responsible for such high binding constants of **2**/(**3a**–**d**) adducts compared to that of **1**/(**3a**–**d**) adducts in acetonitrile.

4. Conclusion

Charge transfer bands between two newly synthesized sterically hindered crown ethers (**1** and **2**) and four BBIM-propane salts in acetonitrile were observed in the UV region. Analyzing the CT parameters, it is found that least substituted axel (**3a**) form most stable complex with both the crowns. **3a** forms stable ground and excited state isosbestic and iso-emissive with both crowns. But the binding ability or association constant of adducts (**1/3a** and **2/3a**) demonstrated that **2/3a** complex was markedly stable compared to that of **1/3a**, both in the ground and excited states. Monte Carlo global minimum searching of adducts in gas phase ultimately concludes that steric factor determined the stability of crown-axel externally H-bonded adducts.

Acknowledgments

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References

[1] (a) S.J. Cantrill, A.R. Pease, J.F. Stoddart, J. Chem, Soc. Dalt. Trans. (2000) 3715–3734;
(b) V. Lamare, D. Haubertin, J. Golebiowski, J.F. Dozol, J. Chem. Soc. Perkin Trans. 2 (2001) 121–127;
(c) S.J. Loeb, J. Tiburcio, S.J. Vella, J.A. Wisner, Org. Biomol. Chem. 4 (2006) 667–680;
(d) V. Valderrey, E.C. Escudero-Adan, P. Ballester, J. Am. Chem. Soc. 134 (2012) 10733–10736.
[2] (a) H.V. Ly, J. Moilanen, H.K. Tuononen, M. Parvez, R. Roesler, Chem. Commun. 47 (2011) 8391–8393;
(b) A. Iordache, M. Oltean, A. Milet, F. Thomas, B. Baptiste, E. Saint-Aman, C. Bucher, J. Am. Chem. Soc. (2012) 2653–2671;
(c) H. Li, H. Zhang, Q. Zhang, Q.W. Zhang, D.H. Qu, Org. Lett. 14 (2012) 5900–5903.
[3] H.V. Huynh, W. Sim, C.F. Chin, Dalton Trans. 40 (2011) 11690–11692.
[4] (a) J.M. Mahoney, R. Shukla, R.A. Marshall, A.M. Beatty, J. Zajicek, B.D. Smith, J. Organomet. Chem. 67 (2002) 1436–1440;
(b) N.K. Jena, N.A. Murugan, J. Phys. Chem. C 117 (2013) 25059–25068.
[5] (a) N.D. Suhan, S.J. Loeb, S.H. Eichhorn, J. Am. Chem. Soc. 135 (2013) 400–408;
(b) J. Fan, M. Hu, P. Zhan, X. Peng, Chem. Soc. Rev. 42 (2013) 29–43.
[6] (a) P.C. Junk, New J. Chem. 32 (2008) 762–773;
(b) P.C. Junk, J.W. Steed, J. Chem. Soc. Dalton Trans. (1999) 407–414.
[7] (a) W. Jiang, K. Nowosinski, N.L. Low, E.V. Dzyuba, F. Klautzsch, A.S. fer, J. Huuskonen, K. Rissanen, C.A. Schalley, J. Am. Chem. Soc. (2012) 1341860–1341868;
(b) S.J. Vella, J. Tiburcio, S.J. Loeb, Chem. Commun. (2007) 4752–4754;
(c) S.J. Loeb, D.A. Tramontozzi, Org. Biomol. Chem. 3 (2005) 1393–1401;
(d) S.I. Pascu, T. Jarrosson, C. Naumann, S. Otto, G. Kaiser, J.K.M. Sanders, New J. Chem. 29 (2005) 80–89;
(e) S. Saha, P. Ghosh, J. Chem. Sci. 124 (2012) 1229–1237;
(f) R.C. Knighton, P.D. Beer, Chem. Commun. 50 (2014) 1540–1542.
[8] S. Saha, J.F. Stoddart, Chem. Soc. Rev. 36 (2007) 77–92.
[9] T. Chaudhuri, A. Karmakar, S. Ghosh, C. Mukhopadhyay, S. Pal, M. Banerjee, J. Lumin. 161 (2015) 164–173.
[10] C. Mukhopadhyay, S. Ghosh, R.J. Butcher, Arkivoc ix (2010) 75–96.
[11] D. Pal, K. Kundu, S. Nayak, S. Bhattacharya, Spectrochim. Acta A 138 (2015) 958–963.
[12] S. Ghosh, T. Chaudhuri, C. Mukhopadhyay, RSC Adv. 4 (2014) 18835–18841.
[13] A. Karmakar, T. Chaudhuri, S. Mula, S. Chattopadhyay, Spectrochim. Acta A 137 (2015) 1258–1264.
[14] I.R. Gould, D. Noukakis, L. Gomez-Jahn, R.H. Young, J.L. Goodman, S. Farid, Chem. Phys. 176 (1993) 439–456.
[15] C. Mukhopadhyay, S. Ghosh, A.M. Schmiedekamp, Org. Biomol. Chem. 10 (2012) 1434–1439.
[16] S. Ghosh, T. Chaudhuri, E. Padmanaban, C. Mukhopadhyay, (communicated)
[17] H.A. Benesi, J.H. Hildebrand, J. Am. Chem. Soc. 71 (1949) 2703–2707.
[18] T. Chaudhuri, D. Goswami, M. Banerjee, S. Chattopadhyay, S.K. Nayak, J. Lumin. 130 (2010) 1750–1755.