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Influence of hydrogen bonding on 'soft' coordination geometries: further examples

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Abstract

The X-ray crystal structures of five new crown ether complexes of Na^+ and Ag^+ are reported, namely: [Ag(18-crown-6)(H_2O)(NO_3)] (**4**), [Ag(18-crown-6)(CF_3SO_3)] (**5**), [Na(18-crown-6)$(H_2O)_2$](CF_3SO_3)·18-crown-6 (**6**), [Na(18-crown-6)$(MeOH)_2$](BPh_4) (**7**), [Na_2(dibenzo-30-crown-10)(H_2O)(MeOH)]$(BPh_4)_2$·MeOH (**8**). Compounds **4** and **7** exhibit intramolecular $OH\cdots O_{crown}$ hydrogen bonds resulting in marked distortions of the complex in order to simultaneously maximise ion–dipole interactions with the metal centre and satisfy the hydrogen bonding requirements of the system. Compound **6** exhibits intermolecular hydrogen bonding interactions to the uncomplexed crown ether, while compound **5** does not contain any hydrogen bonding protons but forms a surprising intermolecular *pseudo*-agostic $CH_2\cdots Ag$ interaction.

Keywords: Interaction; Hydrogen bonding; Proton; Intramolecular

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1. Introduction

There is a growing body of work that highlights the influence that 'crystal packing forces' can exert on the conformational and geometric characteristics of crystal structures [1–5]. Non-covalent interactions such as hydrogen bonds are of particular importance because of their strong and highly directional nature [6–8]. Cases where *intramolecular* interactions are observed are of particular interest because intramolecular hydrogen bonds observed using diffraction techniques in the solid state are likely to persist in the solution phase because, unlike intermolecular interactions, they are not subject to solution concentration effects. The ultimate example of the importance of comparability of solution and solid state interactions is in the study of the tertiary structure of proteins and other biological molecules [9–11].

We have published a number of studies on the influence of strong hydrogen bonding on metal coordination geometry in crown ether complexes [1,3,4]. The crown ethers, with their poor hydrogen bond donor and good acceptor characteristics, coupled with the conformational rigidity lent by the macrocyclic ring, represent excellent model compounds for systematic studies on the competition between covalent, coordination and hydrogen bonding interactions. In particular we have recently reported a series of non-complementary 18-crown-6 complexes of Na^+ such as [Na(18-crown-6)(H_2O)X] (X = NO_3, **1**; ClO_4, **2**; ReO_4, **3**) in which the metal ion is ostensibly too small to fit the macrocyclic cavity [3]. As a result, additional intramolecular, stabilising hydrogen bonding interactions occur between the coordinated aqua ligand and the crown ether. We have also demonstrated the general importance of hydrogen bonding in crown ether complexes by an extensive survey of compounds in the Cambridge Structural Database (CSD) [5]. We now report the preparation and structures of several additional examples which strongly highlight the paramount importance of strong hydrogen bonding interactions in determining overall structure in these types of 'soft' system. By the term soft we understand a metal complex possessing a non-rigid

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coordination geometry with limited orbital contribution to the bonding.

2. Results and discussion

Co-crystallisation of silver(I) nitrate with 18-crown-6 in aqueous solution in the dark results in the formation of large, colourless crystals of [Ag(18-crown-6)(H_2O)(NO_3)] (**4**), Fig. 1. Remarkably, the compound is isostructural with the Na^+ complex [Na(18-crown-6)(H_2O)(NO_3)] (**1**) previously reported by us [3]. The strong $OH\cdots O_{crown}$, $OH\cdots O_{nitrate}$ interactions observed in **1** are also present in **4**, as is the structurally important $CH\cdots O_{nitrate}$ interaction (though this is longer in **4**). Comparing the $OH\cdots O_{crown}$ distances the $O\cdots O$ contact in **4** is somewhat shorter than in **1** (3.00 vs. 3.11 Å), while the $OH\cdots O_{nitrate}$ distances are nearly identical in the two systems. The shortest Ag–O distances is 2.58 Å, rather longer than the shortest Na–O distance of 2.47 Å consistent with a larger ionic radius for Ag^+. The M–OH_2 distances are similar in the two compounds, while the Ag^+ ion forms a rather longer contact to the nitrato ligand than Na^+. Generally, however, in both complexes the metal cation apparently behaves as a spherical positive charge and despite the differences in electronic (hard/soft [12]) character between Na^+ and Ag^+, the bond distances to Ag^+ are generally similar to the Na^+ analogue. It is clear that the geometry of the complex is governed by geometric and steric requirements and the hydrogen bonding preferences of the ligands. The larger size of Ag^+ allows the formation of a shorter intramolecular hydrogen bond.

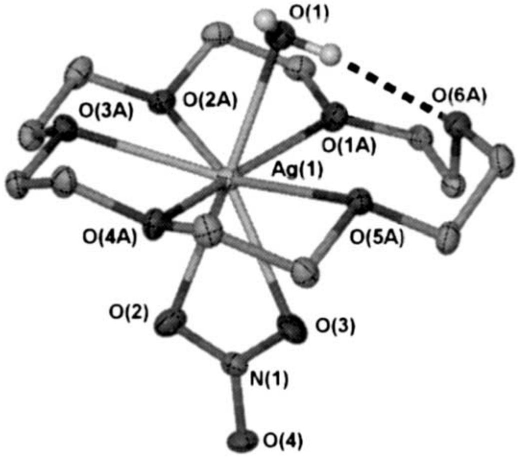

Fig. 1. X-ray crystal structure of [Ag(18-crown-6)(H_2O)(NO_3)] (**4**), isostructural with the Na^+ analogue (CH atoms omitted for clarity) [3]. The hydrogen bonding scheme is completed by an intermolecular interaction to the uncoordinated nitrate oxygen atom on an adjacent molecule. Selected bond lengths: Ag(1)–O(1) 2.3826(15), Ag(1)–O(3) 2.4620(15), Ag(1)–O(3A) 2.5753(13), Ag(1)–O(4A) 2.6391(13), Ag(1)–O(2) 2.6432(16), Ag(1)–O(1A) 2.6644(13), Ag(1)–O(2A) 2.7212(14), Ag(1)–O(5A) 3.1639(14), Ag(1)–O(6A) 3.5525(14) Å; hydrogen bond distances: O(1)···O(1A) 2.964(2), O(1)···O(4)′ 2.821(2) Å.

Contrasting results were obtained in the case of silver(I) and sodium(I) triflate, however. Reaction of $AgCF_3SO_3$ with 18-crown-6 gives the 1:1 complex [Ag(18-crown-6)(CF_3SO_3)] (**5**), whereas $NaCF_3SO_3$ yields crystals of formula [Na(18-crown-6)(H_2O)$_2$](CF_3SO_3)·18-crown-6 (**6**) in which the Na^+ ion is hydrated and the crystal includes an additional molecule of free 18-crown-6 which acts as a hydrogen bond acceptor. Related examples are known [5]. This difference in behaviour might be attributed to a difference in the hydration free energies of the two metal cations, although more probably results from the differences in crystallisation conditions, with an excess of crown ether being present in the case of **6**.

The structure of anhydrous **5** shows that even in the absence of hydrogen bonding interactions the crown ether does not adopt the common D_{3d} structure seen in a variety of other complexes. The structure is very different to **4**, in that Ag–O_{crown} distances cover a much more narrow range and may all be considered 'bonding' (2.60–2.78 Å; *cf.* 2.58–3.55 Å in **4**) consistent with the fact that the crown ether is not now distorting in order to accommodate the intramolecular hydrogen bond. The Ag^+ ion is coordinated to one oxygen atom of the triflate anion on one face while the distortion of the crown ether appears to minimise the exposed surface of the Ag^+ ion on the opposite side of the molecule, Fig. 2(a). Interestingly the remaining exposed surface of the silver ion forms a short contact to both H atoms of a CH_2 group on a neighbouring molecule (Fig. 2(b)) with the $C\cdots Ag$ distance being 3.37 Å. The $H\cdots Ag$ contacts are 2.84 and 2.98 Å using a standard X-ray CH bond length of 0.99 Å. This results in the packing of the molecules into a chiral 2_1 helix and the structure spontaneously resolves in space group $P2_12_12_1$. Such interactions have been termed intermolecular *pseudo*-agostic (IPA) [2]. For comparison the non-bifurcated IPA interaction in ($HNMe_3$)[Co(CO)$_4$] results in an $N\cdots Co$ distance of 3.38 Å while the $H\cdots Co$ distance is 2.37 Å from X-ray data [13]. A neutron structure of the analogous triethyl ammonium species gives $N\cdots Co$ 3.666 Å and $H\cdots Co$ 2.611 Å [14].

Complex **6** is a marked contrast to **4** and the $NaNO_3$ species **1** in that the presence of the additional crown ether obviates the need for intramolecular hydrogen bonding. Thus all $NaOH_2\cdots O_{crown}$ interactions are intermolecular with the uncomplexed crown ether acting as the hydrogen bond acceptor, Fig. 3. Also, as with other non-coordinating anions such as N_3^- and I_3^- the sodium cation is bound axially to two aqua ligands rather than to the counter anion [3]. The structure comprises an infinite hydrogen bonded chain with alternating [Na(crown)(H_2O)$_2$]$^+$ and free crown ether

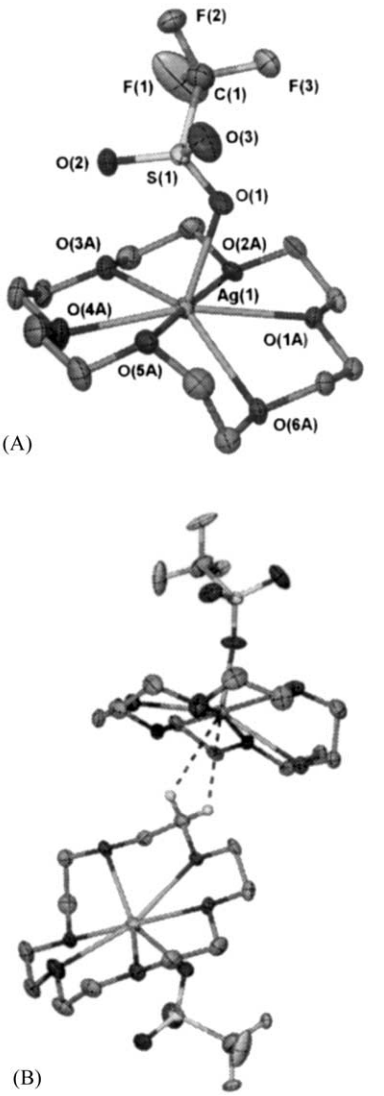

Fig. 2. (a) X-ray crystal structure of [Ag(18-crown-6)(CF_3SO_3)] (**5**) (CH atoms omitted for clarity). Selected bond lengths: Ag(1)–O(1) 2.352(3), Ag(1)–O(4A) 2.604(3), Ag(1)–O(3A) 2.614(3), Ag(1)–O(1A) 2.678(3), Ag(1)–O(5A) 2.721(3), Ag(1)–O(2A) 2.759(2), Ag(1)–O(6A) 2.780(3) Å. (b) Short IPA $CH_2\cdots$Ag contacts in **5**. C···Ag 3.373 Å, H···Ag 2.84 and 2.98 Å.

units. As a result of the absence of intramolecular hydrogen bonding, the Na^+ ion is situated more centrally in the 18-crown-6 ring than in **1**. There is a particular contrast to the highly unsymmetrical [Na(18-crown-6)(H_2O)$_2$]N_3^- (**9**) which forms two intramolecular OH···O_{crown} hydrogen bonds. Na^+–O distances range from 2.64–3.07 Å in **6** and 2.43–3.23 Å in **9** [3].

We and others [3,15] have had some success in minimising the influence of the counter anion on hydrogen bonding features through the use of the large, non-coordinating tetraphenyl borate anion. Thus reaction of $NaBPh_4$ with 18-crown-6 in water leads to the interesting binuclear species [Na_2(H_2O)$_2$(μ-H_2O)(18-crown-6)$_2$](BPh_4)$_2$ (**10**). We now find that this same reaction carried out in methanol solution instead of water yields an analogous methanol solvate, [Na(18-crown-6)(MeOH)$_2$](BPh_4) (**7**) exhibiting a markedly shorter intramolecular OH···O hydrogen bond than in **1** and **4** in which the conformation for the crown ether is highly optimised for this interaction, Fig. 4, presumably because there is now no intermolecular hydrogen bonding. As a consequence the Na^+ ion is situated far to one side of the cavity with the one non-bonding Na–O distance being significantly longer than the remaining five (bonding Na–O 2.50–2.76 Å; non-bonding 3.43 Å). Interestingly, while one coordinated methanol molecule forms such a strong hydrogen bond, the other is not involved in any short hydrogen bond type contacts, although long interactions to other crown oxygen atoms and to the aryl rings of the counter anion are present (Fig. 5).

Finally, the large counter anion BPh_4^- has also allowed us to isolate a further Na^+ complex of the large crown ether dibenzo-30-crown-10. Dibenzo-30-crown-10 is known to form 1:1 ‘wrap-around’ complexes with metals such as K^+, Tl^+ and Ba^{2+} as well as $H_7O_3^+$ [16–19]. With smaller ions such as sodium (as the thiocyanate salt) and H_3O^+ 1:2 complexes are formed, however [20,21]. Unlike [Na_2(NCS)$_2$(dibenzo-30-crown-10)]·H_2O (**11**) [20] however, the present compound [Na_2(dibenzo-30-crown-10)(H_2O)(MeOH)](BPh_4)$_2$·MeOH (**8**) does not contain metal coordinated counter anions. Instead one Na^+ ion is coordinated to water while the other bonds to methanol. Despite this, however, the structures of the crown ethers in **8** and **11** are similar, (although the helical twist of the crown ether is rather different, Fig. 6) and are not influenced by intramolecular hydrogen bonding. The methanol ligand attached to Na(1) hydrogen bonds to another molecule of lattice methanol while the aqua ligand forms an OH···π interaction [22,23] with one of the phenyl groups of a BPh_4^- anion, O···centroid 3.37 Å.

3. Conclusion

This work has shown that intramolecular hydrogen bonding is a major factor in determining the gross structural features of metal complexes with soft coordination geometries. Furthermore the importance of such interactions grows as the influence of competing intramolecular hydrogen bonds diminishes. Unexpectedly we have also demonstrated the existence of a remarkable IPA interaction involving Ag^+ and a crown ether CH_2 group.

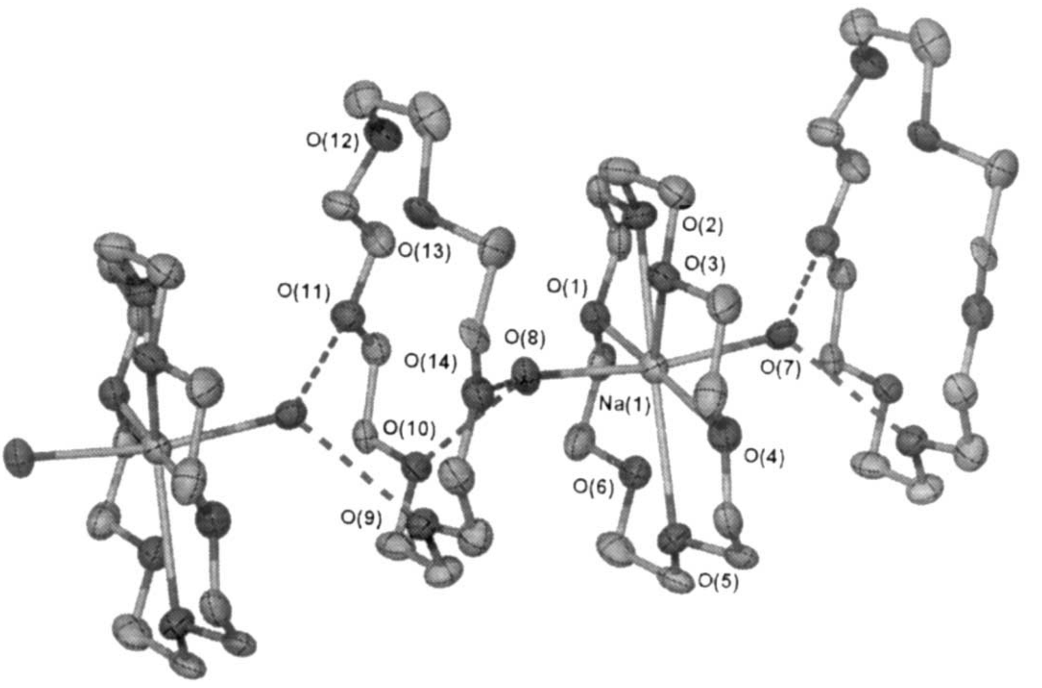

Fig. 3. X-ray crystal structure of a portion of the infinite hydrogen bonded chain formed by the cation in $[Na(18\text{-crown-}6)(H_2O)_2](CF_3SO_3)\cdot 18\text{-crown-}6$ (**6**) showing intermolecular hydrogen bonds to the uncomplexed crown ether (CH atoms omitted for clarity). Selected bond lengths: Na(1)–O(7) 2.280(8), Na(1)–O(8) 2.290(8), Na(1)–O(2) 2.618(8), Na(1)–O(3) 2.636(8), Na(1)–O(4) 2.662(8), Na(1)–O(1) 2.827(9), Na(1)–O(5) 2.925(8). Hydrogen bond distances: O(7)···O(11) 2.863(10), O(7)···O(9) 2.862(9), O(8)···O(10)′ 2.821(10), O(8)...O(14)′ 3.018(10) Å.

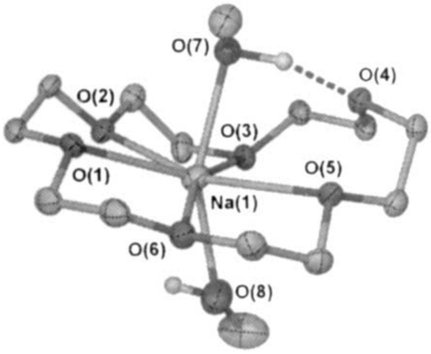

Fig. 4. X-ray crystal structure of the cation in $[Na(18\text{-crown-}6)(MeOH)_2](BPh_4)$ (**7**) showing the short intramolecular hydrogen bond to the crown ether. Selected bond lengths: Na(1)–O(8) 2.328(3), Na(1)–O(7) 2.372(3), Na(1)–O(2) 2.499(3), Na(1)–O(6) 2.500(3), Na(1)–O(1) 2.543(2), Na(1)–O(5) 2.753(3), Na(1)–O(3) 2.763(3) Å. Hydrogen bond distances: O(7)···O(4) 2.792(3) Å.

4. Experimental

4.1. Crystallography

4.1.1. Crystal data for 4

$C_{12}H_{26}AgNO_{10}$, $M = 452.21$, monoclinic, space group $P2_1/n$ (No. 14), $a = 12.1145(4)$, $b = 10.4716(4)$, $c = 13.9884(5)$ Å, $\beta = 103.9090(10)^\circ$, $V = 1722.51(11)$ Å^3, $Z = 4$, $D_c = 1.744$ g cm^{-3}, $F_{000} = 928$, Nonius KappaCCD CCD diffractometer, Mo Kα radiation, $\lambda = 0.71070$ Å, $T = 123(2)$ K, $2\theta_{\max} = 52.0^\circ$, 6453 reflections

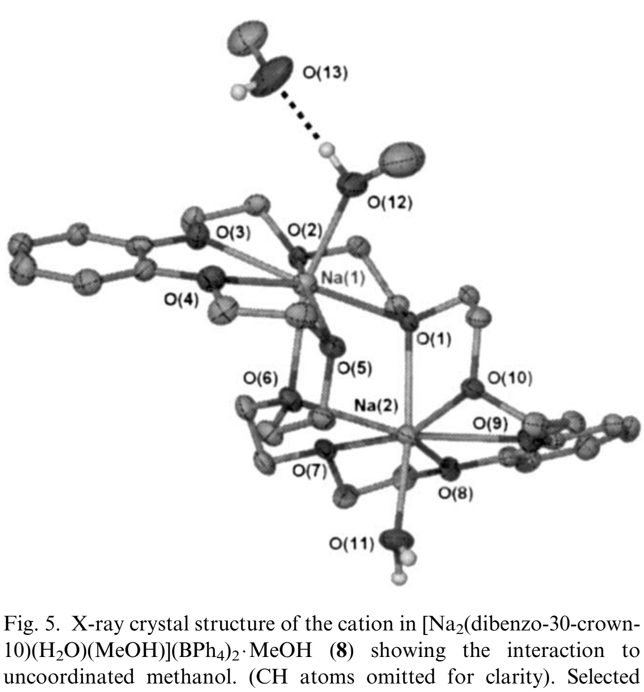

Fig. 5. X-ray crystal structure of the cation in $[Na_2(\text{dibenzo-30-crown-}10)(H_2O)(MeOH)](BPh_4)_2\cdot MeOH$ (**8**) showing the interaction to uncoordinated methanol. (CH atoms omitted for clarity). Selected bond and non-bond distances: Na(1)–O(12) 2.290(4), Na(1)–O(2) 2.398(3), Na(1)–O(6) 2.405(4), Na(1)–O(5) 2.420(3), Na(1)–O(3) 2.502(4), Na(1)–O(4) 2.539(4), Na(1)–O(1) 2.649(4), Na(2)–O(11) 2.319(4), Na(2)–O(10) 2.469(4), Na(2)–O(8) 2.472(4), Na(2)–O(7) 2.482(4), Na(2)–O(9) 2.533(4), Na(2)–O(6) 2.654(4), Na(1)–Na(2) 3.945(3) Å. Hydrogen bond distance: O(12)···O(13) 2.729(6) Å.

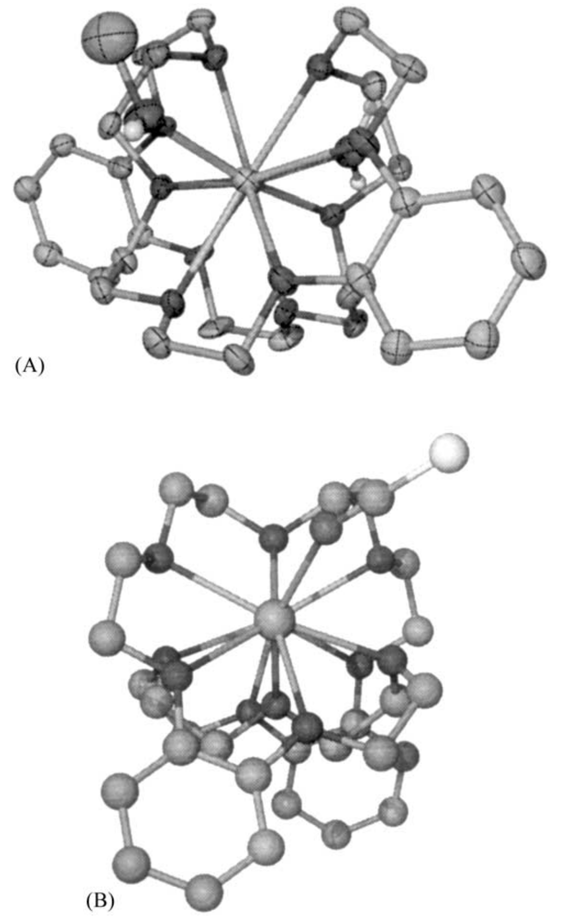

Fig. 6. Comparison of (a) the cation in **8** with (b) [$Na_2(NCS)_2$(dibenzo-30-crown-10)]·H_2O (**11**) (CH atoms omitted for clarity) [20].

collected, 3348 unique ($R_{int} = 0.0218$). The structure was solved and refined using the programs SHELXS-97 [24] and SHELXL-97 [25], respectively. The program X-Seed [26] was used as an interface to the SHELX programs, and to prepare the figures. Final GooF = 1.051, $R_1 =$ 0.0215, $wR_2 = 0.0510$, R indices based on 3062 reflections with $I > 2\sigma(I)$ (refinement on F^2), 226 parameters, 0 restraints. Lp and absorption corrections applied,?$\mu =$ 1.221 mm^{-1}. Other details of crystallographic procedures in our lab have been described previously [19].

4.1.2. Crystal data for 5

$C_{13}H_{24}AgF_3O_9S$, $M = 521.25$, orthorhombic, space group $P2_12_12_1$ (No. 19), $a = 8.0555(2)$, $b = 14.5168(6)$, $c = 16.6781(7)$ Å, $V = 1950.34(12)$ Å^3, $Z = 4$, $D_c = 1.775$ g cm^{-3}, $F_{000} = 1056$, $T = 123(2)$ K, $2\theta_{max} = 52.0°$, 16983 reflections collected, 3818 unique ($R_{int} = 0.0580$). Final GooF = 1.080, $R_1 = 0.0300$, $wR_2 = 0.0651$, R indices based on 3659 reflections with $I > 2\sigma(I)$ (refinement on F^2), 245 parameters, 0 restraints. Lp and absorption corrections applied, $\mu = 1.211$ mm^{-1}. Absolute structure parameter = −0.03(3) [27].

4.1.3. Crystal data for 6

$C_{25}H_{52}F_3NaO_{17}S$, $M = 736.72$, triclinic, space group $P\bar{1}$ (No. 2), $a = 8.5839(17)$, $b = 14.022(3)$, $c = 15.866(3)$ Å, $\alpha = 84.215(3)°$, $\beta = 76.576(3)°$, $\gamma = 75.97°$, $V =$ 1800.1(6) Å^3, $Z = 2$, $D_c = 1.359$ g cm^{-3}, $F_{000} = 784$, $T = 120(2)$ K, $2\theta_{max} = 50.0°$, 10 038 reflections collected, 6198 unique ($R_{int} = 0.1287$). Final GooF = 1.141, $R_1 =$ 0.1534, $wR_2 = 0.3134$, R indices based on 3567 reflections with $I > 2\sigma(I)$ (refinement on F^2), 452 parameters, 12 restraints. Lp and absorption corrections applied, $\mu = 0.186$ mm^{-1}. Crystals proved to be twinned and as a result data precision is poor, however the principal structural features are unambiguous. Atoms C21, C22 and O13 are disordered over 2 sites, each of 50% occupancy.

4.1.4. Crystal data for 7

$C_{38}H_{52}BNaO_8$, $M = 670.60$, monoclinic, space group $P2_1/c$ (No. 14), $a = 14.4147(9)$, $b = 13.5909(6)$, $c =$ 19.4170(15) Å, $\beta = 102.357(4)°$, $V = 3715.8(4)$ Å^3, $Z =$ 4, $D_c = 1.199$ g cm^{-3}, $F_{000} = 1440$, $T = 100(2)$ K, $2\theta_{max} = 50.0°$, 20 938 reflections collected, 6519 unique ($R_{int} = 0.1138$). Final GooF = 1.068, $R_1 = 0.0734$, $wR_2 = 0.1348$, R indices based on 4371 reflections with $I > 2\sigma(I)$ (refinement on F^2), 437 parameters, 0 restraints. Lp and absorption corrections applied, $\mu =$ 0.092 mm^{-1}.

4.1.5. Crystal data for 8

$C_{78}H_{90}B_2Na_2O_{13}$, $M = 1303.10$, triclinic, space group $P\bar{1}$ (No. 2), $a = 11.575(2)$, $b = 15.766(3)$, $c = 19.962(4)$ Å, $\alpha = 95.694(3)°$, $\beta = 96.915(3)°$, $\gamma = 101.547(3)°$, $V =$ 3514.6(12) Å^3, $Z = 2$, $D_c = 1.231$ g cm^{-3}, $F_{000} = 1388$, $T = 120(2)$ K, $2\theta_{max} = 50.0°$, 19 971 reflections collected, 12 285 unique ($R_{int} = 0.1463$). Final GooF = 1.038, $R_1 = 0.0899$, $wR_2 = 0.1491$, R indices based on 6294 reflections with $I > 2\sigma(I)$ (refinement on F^2), 859 parameters, 0 restraints. Lp and absorption corrections applied $\mu = 0.092$ mm^{-1}.

4.2. Preparations

Conditions were chosen to optimise the formation of diffraction quality crystals which generally proved to be highly sensitive to exposure to atmosphere. As a result meaningful yields could not be obtained, but are estimated to be in excess of 50% in each case.

4.2.1. [Ag(18-crown-6)(H_2O)(NO_3)] (4)

Silver(I) nitrate (0.20 g, 1.0 mmol) was dissolved in ethanol (1 cm^3) and mixed with a solution of 18-crown-6 (0.21 g, 1.0 mmol) in ethanol (1 cm^3) and the resulting colourless solution allowed to stand in the dark for 3 weeks resulting in the deposition of the product as colourless needles.

4.2.2. $[Ag(18\text{-crown-}6)(CF_3SO_3)]$ (5)

Silver(I) trifluoromethane sulfonate (0.20 g, 1.0 mmol) was dissolved in ethanol (1 cm^3) and mixed with a solution of 18-crown-6 (0.21 g, 1.0 mmol) in ethanol (1 cm^3) and the resulting colourless solution allowed to stand in the dark for 1 week resulting in the deposition of the product as colourless needles.

4.2.3. $[Na(18\text{-crown-}6)(H_2O)_2](CF_3SO_3)\cdot 18\text{-crown-}6$ (6)

Sodium trifluoromethane sulfonate (0.065 g, 0.18 mmol) was dissolved in distilled water (5 cm^3) and mixed with a solution of 18-crown-6 (0.21 g, 1.0 mmol) in distilled water (5 cm^3) and the resulting colourless solution allowed to stand in the dark for 3 months resulting in the deposition of the product as colourless needles.

4.2.4. $[Na(18\text{-crown-}6)(MeOH)_2](BPh_4)$ (7)

Sodium tetraphenylborate (0.052 g, 0.15 mmol) was dissolved in distilled water (1 cm^3) and mixed with a solution of 18-crown-6 (0.040 g, 0.20 mmol) in methanol (1 cm^3) resulting in the formation of an immediate white precipitate. This solid was redissolved in methanol (10 cm^3) resulting in the deposition of the product as colourless plates over a period of minutes.

4.2.5. $[Na_2(\text{dibenzo-30-crown-10})(H_2O)(MeOH)](BPh_4)_2\cdot MeOH$ (8)

Sodium tetraphenylborate (0.086 g, 0.25 mmol) was dissolved in methanol (1 cm^3) and mixed with a solution of dibenzo-30-crown-10 (0.034 g, 0.012 mmol) in methanol (1 cm^3) resulting in the formation of an immediate white precipitate. This solid was redissolved in methanol (5 cm^3) resulting in the deposition of the product as brownish prisms over a period of 1 week.

5. Supplementary material

Atomic coordinates, bond lengths and angles and thermal parameters have been deposited at the Cambridge Crystallographic Data Centre, CCDC Nos. 191142–191146 for **4**–**8**. Copies of this information can be obtained free of charge from the Director, CCDC 12 Union Road, Cambridge, CB2 1EZ, UK (fax: +44-1223-336033; e-mail: deposit@ccdc.cam.ac.uk or http://www.ccdc.ac.uk).

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