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Crystal structure of hydrates of imidazolium salts

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ABSTRACT

Single crystal X-ray structures of three imidazolium salts were examined. In contrast to imidazolium salt **1** possessing an ester group which created a network of C—H···halide–anion interactions with a linear array of imidazolium and the corresponding counter anions, unique network structures were observed in imidazolium salts **2** and **3** with long alkyl chains and with carboxy moieties, respectively. Water molecules were incorporated in their H-bonding networks. Water molecules were wedged into the two neighboring halide anions to create square units which acted as a bridge to connect the two adjacent C—H···halide–anion networks of imidazolium moieties and counter anions.

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1. Introduction

Recently, much attention has been paid to the chemistry of imidazolium salts as ionic liquids [1–6] and ionic liquid crystals [7,8]. Imidazolium-based ionic liquids are the most commonly used ionic liquids for extraction and reaction solvents because of their nonflammability and nonvolatility. Imidazolium salts are also utilized as ionic liquid crystalline materials. Stable liquid crystals could be generated from imidazolium salts substituted with long alkyl chains due to an efficient microphase separation of ionic cores (imidazolium moieties) from flexible lipophilic alkyl chains. They are investigated as potential ion conductive materials [9-11] and lithium-ion batteries [12]. X-ray crystallographic studies of imidazolium salts have been studied in order to design novel functionalized ionic liquids [13-20]. We are interested in the arrangement of counter anions for elucidation of the assembled structures in ionic liquid crystals. However, the examples of their structural elucidation are limited [21-25]. In the course of our study on imidazolium-based ionic liquid crystals [26], we have found and examined the crystal structure of the hydrated imidazolium salts. In this paper, we report on the array of the imidazolium cations and the corresponding counter anions associated with water molecules.

In some cases, the way of packing in the crystal structures of imidazolium salts involves clipping of counter anions with the two adjacent cationic imidazolium rings. Counter anions are located near the surface of imidazolium rings via ionic interactions. The ionic layer thus created is separated by the layers of aliphatic substituents [21,22,27-29] (Fig. 1a). This microphase separation is applied to the generation of stable ionic liquid crystals. The other type of packing includes C—H···halide–anion interacted networks, the association of hydrogen atoms at the 2- and 4-positions of the imidazolium moiety with the counter anions. Imidazoliums and counter anions are aligned alternately in a horizontal way [17] (Fig. 1b).

The network structure we will discuss here involves the incorporation of water molecules. There are a few reports on single crystal X-ray structures of hydrated imidazolium halides [30-34]. Water molecules were incorporated in their H-bonding networks. We found a unique arrangement of water molecules. Water molecules were wedged into the two neighboring halide anions to create four-membered square units which acted as bridges to connect the two adjacent C-H···halide-anion interacted networks of imidazolium moieties and counter anions (Fig. 1c). A similar type of the hydrate of the imidazolium salt was reported on the imidazolium substituted with a long mono-alkyl chain [33]. An interesting water clusters were reported in the crystal structures of metal complexes of zwitterionic type imidazoliums [18,35]. Apart from imidazolium salts, halide anions associate with water to form halide-water clusters. Supramolecular assembly of chloride-water tapes and bromide-water chains were reported in the crystal structure of terpyridine salts [36]. An interesting dimeric capsule of an arene based tripodal amide receptor was formed using fluoride-water clusters as a template [37]. Chloride-water clusters were generated in MOFs (Metal Organic Frameworks) with free carboxylic acid sites [38].



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Fig. 1. Schematic representation of three types of network structures of imidazolium salts in their crystal structures. Counter anions and water molecules are indicated by pink and sky-blue spheres, respectively. (a) A sandwich structure in which counter anions are clipped by the neighboring imidazolium moieties, (b) networks of imidazolium-counter ion pairs in a horizontal way, and (c) networks with incorporation of water molecules via H-bonding. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

2. Experimental

2.1. General

All the reagents and solvents employed were commercially available and used as received without further purification. X-ray diffraction data for the crystals were measured on CCD diffractometers. Data collections were carried out at low temperature [150 K for **1** and **3**·(H₂O)₂, and 100 K for **2**·H₂O] by using liquid nitrogen. All structures were solved by direct methods SHELXS-97 [39] and the non-hydrogen atoms were refined anisotropically against F^2 , with full-matrix least squares methods SHELXL-97 [39]. Hydrogen atoms were included as their calculated positions. The position of hydrogen atoms of a water molecule in the crystals of **2**·H₂O were determined based on the electronic density distribution. About a water molecule in the crystals of **3**, the position of hydrogen atoms were not calculated. Crystal data for **1** (CCDC 819420), **2**·H₂O (CCDC 819422), and **3**·(H₂O)₂ (CCDC 819421) are presented in Table 1.

2.2. Synthesis

The imidazolium salts **1** and **3** were prepared by conventional methods described below. The known salt **2** was prepared according to the literature [40].

2.3. 3-(2-Ethoxy-2-oxoethyl)-1-(3,4,5-trimethoxybenzyl)-1Himidazol-3-ium bromide (1)

A mixture of 1-(3,4,5-tris(methoxy)benzyl)imidazole (0.10 g, 0.40 mmol) and ethyl 2-bromoacetate (0.13 mL, 1.2 mmol) in acetonitrile (10 mL) was refluxed for 12 h at 90 °C. The solvent was removed under reduced pressure. The mixture was purified by column chromatography on silica gel (eluent: CHCl₃/MeOH = 9/1) to give **1** (0.14 g, 0.34 mmol) in 84% yield as a white powder. Single crystals were obtained by recrystallization from chloroform/acetonitrile. Mp. 142–144 °C: ¹H NMR (300 MHz, CDCl₃) δ 1.32 (t, *J* = 7.1 Hz, 3H), 3.84 (s, 3H), 3.90 (s, 6H), 4.28 (q, *J* = 7.1 Hz, 2H), 5.42 (s, 2H), 5.43 (s, 2H), 6.76 (s, 2H), 7.30 (t, *J* = 1.4 Hz, 1H), 7.41 (t, *J* = 1.4, 1H), 10.57 (s, 1H): ¹³C NMR (75 MHz, CDCl₃) δ 14.42, 50.73, 54.15, 57.03, 61.21, 63.40, 106.76, 122.00, 124.07, 128.54, 138.26, 139.08, 154.27, 166.44: IR(KBr) v 3172, 3110, 2985, 2841, 1739, 1560, 1510, 1430, 1235, 1163: HRMS (ESI) calcd for C₁₇H₂₃O₅N₂ [M–Br]⁺ 335.1601, found 335.1595.

2.4. 1,1'-(1,4-phenylenebis(methylene))bis(3-(carboxymethyl)-1Himidazol-3-ium) bromide (3)

A mixture of 1,1'-(1,4-phenylenebis(methylene))bis(3-(2-eth-oxy-2-oxoethyl)-1*H*-imidazol-3-ium) bromide (0.200 g, 0.35 mmol) in 1 M aqueous HCl solution (30 mL) was refluxed for 30 min. The solvent was removed under reduced pressure and the remaining solid was washed with acetone and THF to give **3** (0.18 g, 0.34 mmol) as a white powder in 98% yield. Single crystals were obtained by recrystallization from water with diffusion of acetone vapor. Mp. > 270 °C (dec.): ¹H NMR (300 MHz, D₂O) δ 4.97 (s, 4H), 5.34 (s, 4H), 7.34 (s, 4H), 8.80 (s, 2H): ¹³C NMR (75 MHz, D₂O) δ 50.53, 52.95, 122.67, 124.34, 129.78, 134.74, 137.36, 170.43: IR (KBr) ν 3160, 3140, 3120, 3026, 2767, 2681, 2575, 2485, 1733, 1567, 1396, 1199, 1170 cm⁻¹: MS (ESI) calcd for C₁₈H₁₉O₄N₄ [M-2Br-H]⁺ 355.1401, found 355.1399.

3. Results and discussion

The structures of Imidazolium salts **1–3** examined are shown in Scheme 1. The salts **1** and **2** possess phenyl group substituted with trialkoxy groups. The latter is known to show liquid crystallinity

Table 1
Crystallographic data for imidazolium salts 1–3.

Salt	1	2 ⋅H ₂ O	$3 \cdot (\mathrm{H}_2\mathrm{O})_2$
Formula	C17H23BrN2O5	C47H87CIN2O4	$C_{18}H_{24}Br_2N_4O_6$
Crystal system	Triclinic	Triclinic	Triclinic
Space group	P-1	P – 1	P-1
a (Å)	8.8843(9)	7.209(4)	7.0222(8)
b (Å)	10.8379(11)	8.242(5)	8.6568(10)
c (Å)	11.1756(11)	43.03(2)	9.1506(11)
α(°)	104.141(1)	85.385(7)	75.440(1)
β (°)	107.610(1)	87.767(7)	84.095(1)
γ(°)	103.817(1)	68.883(6)	87.955(1)
V (Å ³)	935.90(16)	2377(2)	535.51(11)
$D_c ({\rm Mg}{\rm m}^{-3})$	1.474	1.089	1.712
Ζ	2	2	1
T (K)	150	100	150
$R_1 [I > 2\sigma(I)]$	0.0300	0.0624	0.0508
$wR_2 [I > 2\sigma(I)]$	0.0804	0.1639	0.1588

[40,11]. The salt 3 has two imidazolium moieties. Each substituted with a carboxymethyl group. Single crystals suitable for X-ray analysis were obtained for all these salts. Single crystals of 1 and 3 were obtained from water pervaded with acetone vapor. Recrystallization was carried out from chloroform/acetonitrile (containing trace amounts of water) for 2. The salts 2 and 3 were obtained as monohydrate and dihydrate, respectively. Table 1 shows their crystallographic data. Fig. 2 shows the ORTEP diagram and the H-bonding networks observed in the crystal structure of 1 in which imidazolium moieties and bromine anions are aligned alternately. The acidic hydrogen atoms of the imidazolium create the network of $C-H\cdots$ Br interaction in the direction of the *a*-axis. The C···Br atomic distances are 3.46 and 3.51 Å for the interactions involving the hydrogen atoms at the 2- and 4-position, respectively. The resulting layers created by this H-bonding are packed in an anti-parallel manner. The packing pattern belongs to the one as aforementioned schematically in Fig. 1a. The $C-H\cdots$ Br interaction is also observed for the phenyl and methyl hydrogen atoms. The C...Br atomic distances are 3.81 and 3.78 Å for hydrogen atoms of the phenyl and methyl groups, respectively.

Even with three long alkyl chains the salt **2** gave single crystals. In contrast to the crystal structure of **1**, the salt **2** showed a different network structure. It contained an equimolar amount of water molecules. Water molecules were incorporated in the H-bonding networks. Fig. 3a and b shows its ORTEP and packing diagrams, respectively. Water molecules are wedged into the two neighboring halogen anions via the O-H…Br interaction to create a square unit as depicted schematically in Fig. 1b.

This unit is located alternately with imidazolium to create an ionic layer. This ionic layer was surrounded by lipophilic layers created by long alkyl chains. Lamellar type bilayers are constructed as a whole. Similar lamellar type crystal structure was reported in benzimidazole substituted with two dodecyl groups [30]. It is known that **2** is a thermotropic liquid crystalline material exhibiting a hexagonal columnar liquid crystal phase [11,40]. It forms a disc-like structure by self-assembling in a liquid crystal phase. An expecting liquid crystal phase from the X-ray structure of **2** is a smectic phase. This discrepancy could be originated in the thermal motion of molten long alkyl chains in its liquid crystal phase.



Scheme 1. Chemical diagrams of imidazolium salts 1-3.



Fig. 2. Crystal structure of **1**. (a) ORTEP diagram, (b) selected short contacts between bromide anions and C—H hydrogen atoms indicated with green capped sticks, and (c) packing diagram. Bromide anions are shown as red-brown spheres with arbitrary radii in (b) and (c). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)



Fig. 3. Crystal structure of $2 \cdot H_2O$. (a) ORTEP diagram, (b) packing diagram viewed along the *a*-axis showing bromine anions and water molecules in a space-filling model, and (c) a part of the structure showing short contacts observed in the ionic layer in which chloride anions and water molecules are presented in spheres of arbitrary size. The $O-H\cdots Cl$, $C-H\cdots Cl$, and $C-H\cdots O$ interactions are indicated with sky-blue, green, and red capped sticks, respectively. Distances are indicated in Å. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Because of this motion, a fan-shaped structural unit will be created instead of the rigid rectangular plate in its crystalline state. Several short contacts are observed in the ionic layers. Fig. 3c represents a part of the structure of **2** to show them. The O–H…Cl, C–H…Cl, and C–H…O interactions are indicated with sky-blue, green and red capped sticks, respectively. The observed distances for the O…Cl, C…Cl, and C…O are 3.18, 3.50–3.70, and 3.12–3.52 Å respectively. The C–H… π interaction [41,42] is also observed between the trialkoxy substituted phenyl ring and the adjacent methyl hydrogen atom. The edge-to-face interaction takes place with the distance of 2.60 Å between the centroid of the phenyl ring and the adjacent methyl hydrogen atom.

Prior to our study, single crystal X-ray structures of imidazolium dicarboxylic acids were reported by Dyson et al. [17,18]. They found polymeric networks created by COOH···X interactions in the crystals. In contrast to their work, we obtained imidazolium carboxylic acid **3** as dihydrate. Fig. 4a shows its ORTEP diagram. The molecule has a zigzag shape. Two carboxy moieties direct towards the opposite directions each other, which makes it possible to create linear polymeric networks by linking. The salts are linked with water–bromide–water linkage (Fig. 4b). The resulting network showed the similar pattern as observed in the crystal structure of **2**·H₂O. Two molecules of water and bromide anions are united to create a square unit which behaves as linkers resulting in the array of the salt **3**·(H₂O)₂ via water–carboxylic acid H-bonding. The distances between bromide anions and oxygen atoms of water molecules are 3.15 and 3.14 Å which are 9.5% and 9.8% shorter than the sums of their van der Waals radii, respectively. Recently, the



Fig. 4. Crystal structure of $3 \cdot (H_2O)_2$. (a) ORTEP diagram, (b) H-bonded linear network structure, and (c) a part of the crystal structure showing short contacts. The $0 \cdot \cdot Br$, $C-H \cdot \cdot Br$, $O-H \cdot \cdot O$, $C=0 \cdot \cdot H$ interactions are indicated with sky-blue, green, blue, and red capped sticks, respectively. Oxygen atom and bromide anion are indicated by a red and a red-brown sphere of arbitrary sizes, respectively. The distances are indicated in Å unit. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

importance of a new manner of interaction by which water affects biomolecular behaviors, called halogen–water–hydrogen bridge (XWH bridge), has been emphasized [43,44]. In this bridge one H-bonding in water mediated H-bond bridge is replaced by halogen bonding (X-bonding). The XWH bridges stabilize biomolecular conformations and in mediation of protein–protein, protein–nucleic acid, and receptor–ligand recognition and binding. Since water molecules are H-bonded with neighboring carboxy moieties in $3 \cdot (H_2O)_2$, such XWH bridges could play a significant role in the assembling of imidazolium salts although bromide anions were involved instead of bromine atoms. Fig. 4c presents a part of the crystal structure to show the short contacts observed in the ionic region. In the figure, the $O \cdots Br$, $C - H \cdots Br$, $O - H \cdots O$, and $C = O \cdots H$ interactions are indicated with sky-blue, green, blue, and red capped sticks, respectively. The resulting H-bonded chains as shown in Fig. 4b are interwoven via C—H···Br interactions creating the network orthogonal to the chains. The C=O···H interactions between the carbonyl and the benzylic and one of the phenylene hydrogen atoms also create the network in the same direction as for the C—H···Br interactions.

4. Conclusion

In order to elucidate the arrangement of the counter anions in the crystal structure of imidazolium salts we have examined X-ray structures of three types of imidazolium salts and found a novel C—H…halide–anion interacted network in the linear array of the imidazolium and the corresponding counter anion in hydrated imidazolium salts. Water molecules were wedged into the neighboring halide anions to create a halide–water square unit. This unit behaves as a bridge to connect the two adjacent imidazolium– counter anion networks to stabilize their crystal structures.

Supplementary data

CCDC 819420, 819422, and 819421 for compounds **1**, **2**·H₂O, and **3**·(H₂O)₂ respectively, contain the supplementary crystallographic data for this paper. These data can be obtained free of charge via http://www.ccdc.cam.ac.uk/conts/retrieving.html, or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44 1233 336 033; or e-mail: deposit@ccdc.cam.ac.uk.

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