Tetrakis(pentafluoroethyl)gallate, [Ga(C$_2$F$_5$)$_4$]$^−$, Ionic Liquids

Harry Biller,[a] Swantje Lerch,[a] Katharina Tölke,[b] Hans-Georg Stammler,[b] Berthold Hoge,*[b] and Thomas Strassner*[a]

Abstract: We synthesized new imidazolium-based tunable aryl alkyl ionic liquids (TAAILs) with the weakly coordinating tetrakis(pentafluoroethyl)gallate anion, [Ga(C$_2$F$_5$)$_4$]$^−$. Phenyl and phenyl derivatives (2-Me, 4-OMe, 2,4-F) were combined with varying alkyl chain lengths at the imidazolium core leading to TAAILs, which were investigated with regard to their viscosity, conductivity, and electrochemical window and compared to EMIM and BMIM standard cations. Remarkable low viscosities of 29 cP at 25 °C for [BMIM][Ga(C$_2$F$_5$)$_4$] were achieved. However, the EMIM and BMIM gallates show electrochemical instability, releasing pentafluoroethane at a voltage of 1.5 V. The 2-Me-substituted gallate-TAAILs slowly decompose over several weeks, whereas all other gallate-TAAILs showed no decomposition at all. With electrochemical windows of up to 5.15 V and low viscosities in a range of 66–162 cP, the gallate-TAAILs are promising candidates as electrolytes in electrochemical applications.

Introduction

Ionic liquids (ILs) are salts with melting points below 100 °C. They possess unique properties like low viscosity, non-flammability, ionic conductivity, and negligible vapor pressure.[1,2] Depending on the composition of the anionic/cationic species and the alkyl chain length, the physico-chemical properties of ILs can change significantly.[3] While the number of different combinations of anions and cations is growing steadily, the imidazolium heterocycle has established itself as one of the

most common cations in ILs. In addition to their ease of synthesis, they are stable against air and moisture and show a high decomposition temperature.[4–6] Imidazolium based ionic liquids in combination with anions like BF$_4^−$, PF$_6^−$, and bis (trifluoromethane)sulfonimide, [NTf$_2$]$^−$, are commercially available and well-studied in many fields including synthesis,[7] catalysis,[8] material science[9] and batteries.[10]

Tunable aryl alkyl ionic liquids (TAAILs) introduced by our group differ from typical imidazolium based ILs by the incorporation of a phenyl group at one of the nitrogen atoms.[11] This new type of cation can be easily modified with different functional groups at the phenyl ring resulting in increased customizability.[12] Recently, the effect of different anions in TAAILs was reported. The combination with a dicyanamide anion [N(CN)$_2$]$^−$ results in very wide electrochemical windows,[13] while TAAILs with palladate anions gave access to catalytically active ionic liquids.[14] Weakly coordinating anions are well suited for ionic liquids, since positive effects were achieved by reduced ion interactions.[15] New TAAILs with weakly coordinating anions were synthesized previously containing boron as the central atom. The [B(OCH(CF$_3$)$_2$)$_4$]$^−$ anion leads to lower viscosity and melting points in comparison to the [NTf$_2$]$^−$ anion.[16,17]

In this work we present TAAILs featuring the recently introduced tetrakis(pentafluoroethyl)gallate anion, [Ga(C$_2$F$_5$)$_4$]$^−$. This weakly coordinating anion with gallium as the central atom is highly resistant towards aqueous hydrochloric acid or lithium hydroxide, and is therefore well suited for ionic liquids.[18] With this motivation we synthesized gallate-TAAILs containing different phenyl moieties and characterized them by NMR spectroscopy and elemental analysis. Viscosities and conductivities as well as the electrochemical window were also determined for different alkyl chain lengths.

Results and Discussion

Synthesis

The synthesis of the imidazole core structure was performed in a one-pot condensation reaction with glyoxal, formaldehyde, ammonium chloride and different aniline derivatives.[11,19] Quaternization with alkyl halides leads to the respective imidazolium cations **3a**–**18a** with varying alkyl chain lengths, indicated by the number of hydrocarbons (n = 1, 4, 8, 12; Scheme 1). In addition to the unsubstituted phenyl group (Scheme 1, R = H), TAAILs with phenyl derivatives (2-Me, 4-OMe, 2,4-F) were prepared. The ILs **1a** [EMIM][Br] and **2a** [BMIM][Br] were synthesized by quaternization of 1-methylimidazole with 1-bromoethane or 1-bromobutane, respectively. The gallate

[a] H. Biller, S. Lerch, Prof. Dr. T. Strassner
Department of Chemistry and Food Chemistry
Physical Organic Chemistry
Technical University Dresden
Bergstrasse 66, 01069 Dresden (Germany)
E-mail: thomas.strassner@tu-dresden.de

[b] K. Tölke, Dr. H.-G. Stammler, Prof. Dr. B. Hoge
University Bielefeld, Faculty of Chemistry
Center for Molecular Materials
Universitätsstraße 25, 33615 Bielefeld (Germany)
E-mail: b.hoge@uni-bielefeld.de

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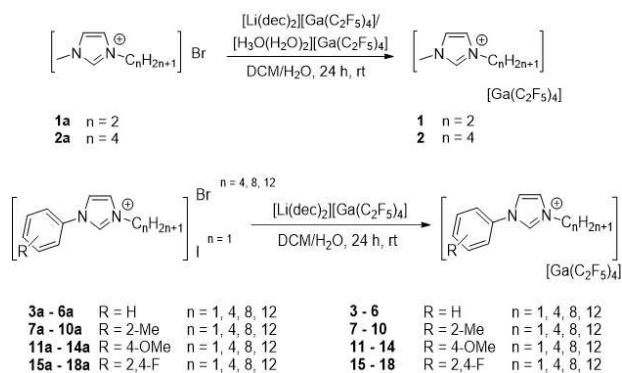
Scheme 1. Synthesis of imidazolium-based ionic liquids with [Ga(C$_2$F$_5$)$_4$]$^-$ as the anion by anion metathesis.

anion was obtained by treatment of [GaCl$_3$(dmap)] (dmap = 4-dimethylaminopyridine) with in situ generated LiC$_2$F$_5$ in diethyl ether. The addition of diethyl carbonate (dec) and removal of all volatile compounds yielded [Li(dec)$_2$][Ga(C$_2$F$_5$)$_4$] as a clear oil. Extraction of the lithium salt dissolved in diethyl ether with aqueous hydrochloric acid and removal of all volatile compounds of the organic layer leads to the oxonium salt [H$_3$O(H$_2$O)$_2$][Ga(C$_2$F$_5$)$_4$].[18]

The anion metathesis was achieved employing [Li(dec)$_2$][Ga(C$_2$F$_5$)$_4$] or [H$_3$O(H$_2$O)$_2$][Ga(C$_2$F$_5$)$_4$] and the respective imidazolium halide in a two-phase system of dichloromethane (DCM) and H$_2$O. After liquid extraction and purification by column chromatography the ILs were obtained in typical yields of 80–95 % (see Supporting Information for details).

All gallate-ILs are resistant towards air and water and can be described as room temperature ionic liquids with melting points below 25 °C, except **1** and **11**, which liquefy above 32 °C and 50 °C, respectively.

Solid State Structure

Crystals of **4**, suitable for an X-ray diffraction study, were grown by in situ crystallization of the melt at 264.4 K in a capillary. **4** crystallizes in the monoclinic space group P2$_1$/n. The molecular structure is shown in Figure 1.

The cation-anion contacts of C1-F12 (305.7(2) pm) and C3'-F15 (308.7(2) pm; C3': x-^{1}/$_2$, 3/2-y, ^{1}/$_2$+z) are shorter than the sum of the van der Waals radii (317 pm) and indicate a weak interaction. The arrangements of the substituents at the nitrogen atoms are trigonal planar (sum of C−N−C angles: 360.0(1)°; 359.8(5)°), which is typical for imidazolium salts.

The structural characteristics of the [Ga(C$_2$F$_5$)$_4$]$^-$ anion do not differ significantly from the literature data.[18]

The electrostatic potentials of the anions [B(CF$_3$)$_4$]$^-$, [Ga(CF$_3$)$_4$]$^-$ and [Ga(C$_2$F$_5$)$_4$]$^-$ are depicted in Figure 2 and clearly demonstrate the weakly coordinating properties of the gallate anion. The red areas represent negative electrostatic potentials at which cation coordination may occur. Repulsive positive
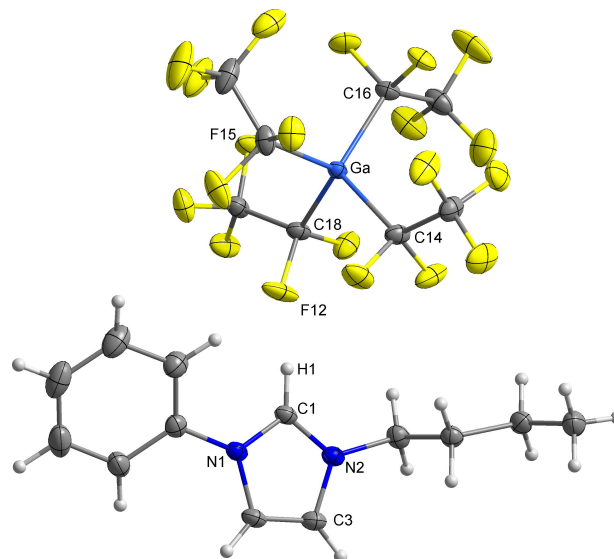
Figure 1. Molecular structure of **4**. Thermal ellipsoids are shown at 50 % probability. Selected bond lengths [pm] and angles [°]: Ga−C18 204.1(1); C1-N1 134.0(2); C1−N2 133.2(2); C14−Ga−C18 101.6(1); C14−Ga−C16 113.2(1).
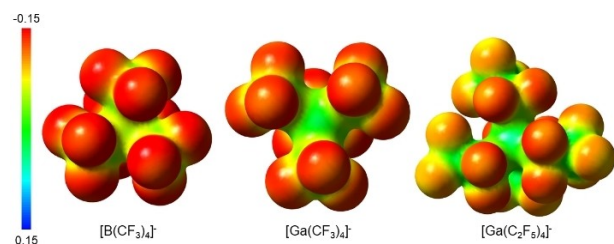
Figure 2. Projection of the calculated electrostatic potential (BP86/SVP) onto a 0.015 e$^-$ Å^{-3} isodensity surface.[20]

electrostatic potentials are shown in blue and non-coordinating areas in green-yellow.

Compared to the anions [B(CF$_3$)$_4$]$^-$ and [Ga(CF$_3$)$_4$]$^-$, the more bulky [Ga(C$_2$F$_5$)$_4$]$^-$ anion accumulates less negative charge on the surface. The CF$_2$-groups of [Ga(C$_2$F$_5$)$_4$]$^-$ are most polarized and thus are able to form coordinating interactions with the counter ion, as obvious from several molecular structures in the literature.[18,21]

Thermal stability

The decomposition temperatures of **2** and **4** were investigated by thermogravimetric analysis (TGA) under argon atmosphere (see Supporting Information, Figures S43–S44). **2** shows a decomposition temperature of 260 °C at 5 wt% mass loss, which is lower in comparison to the BMIM cation with the anions [BF$_4$]$^-$ (399 °C) and [NTf$_2$]$^-$ (419 °C).[22] The decomposition temperature of **4** was slightly higher with 280 °C at 5 wt% mass loss, therefore it can be assumed that the gallate anion has a negative influence on the thermal stability.

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Viscosity measurements

Dynamic viscosities were obtained in 5 K steps from 20 °C to 60 °C. The measurement of **1** starts at 40 °C due to the elevated melting point (32 °C). The dynamic viscosities of **1–6** in centipoise (cP) as a function of the temperature are depicted in Figure 3. Compound **2** showed the lowest viscosity at 25 °C (29.5 cP) within all investigated ILs. At 40 °C, **1** has a slightly increased viscosity (19 cP) than **2** (18 cP). Although EMIM-ILs are usually less viscous than BMIM-ILs ([EMIM][BF$_4$] 43 cP;[23] [BMIM][BF$_4$] 219 cP[5]), the more bulky [Ga(C$_2$F$_5$)$_4$]$^-$ anion diminishes this difference.

As obvious from Figure 3, the size of the cation increases the viscosity. Similarly, the viscosity is concominently influenced by the anion size.[24]

Interestingly, [EMIM][Ga(C$_2$F$_5$)$_4$] shows a low viscosity compared to other EMIM-ILs, despite the larger volume of the anion (Table 1). The viscosity is in the range of EMIM-ILs containing the small [NTf$_2$]$^-$ and the large [Al(OCH(CF$_3$)$_2$)$_4$]$^-$ anion.[25,15a] This apparent contradiction to the general tendency can be rationalized by impeded ion pairing with large weakly coordinating anions as [Ga(C$_2$F$_5$)$_4$]$^-$ and [Al(OCH(CF$_3$)$_2$)$_4$]$^-$ compared to smaller ions. For example, [EMIM][B(CF$_3$)$_4$] is a solid with a melting point of 125 °C.[26]

Regarding the low viscous IL [EMIM][BF$_2$(CN)$_2$], a low volume combined with an efficient charge delocalization may represent a good combination.[24,27]

Synthesized TAAIL-gallates exhibit higher viscosities due to their higher molar mass and reduced ion mobilities by addi-
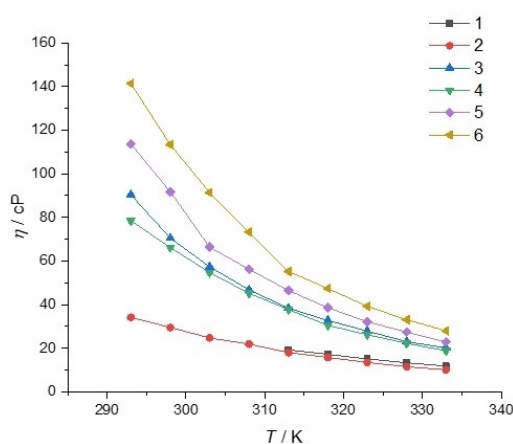
tional π-π interactions of the phenyl groups.[28] As a result, the viscosities of the unsubstituted TAAILs **3–6** lie in a range from 113 cP to 66 cP (25 °C) in the order of the alkyl chain length n = 4 > 1 > 8 > 12. The viscosities of the substituted TAAILs depicted in Figure 4 are following the same pattern in terms of the alkyl chain length, however, they show higher viscosities at all. The 4-OMe substituted ILs (**12-14**) exhibits the highest viscosities between 162–91 cP followed by 2-Me (**7-10**) at 139–77 cP and 2,4-F (**15-18**) at 126–67 cP. Following the Vogel-Fulcher-Tammann equation, viscosities decrease exponentially at higher temperatures and reach less than 50 cP at 60 °C.[29] **11** was left out due to its high melting point.

Electrochemical properties

The electrochemical window of the gallate-ILs was determined by linear sweep voltammetry (LSV) in the pure IL. The measurements were carried out under N$_2$ atmosphere in a conic shaped micro-centrifuge tube with a glassy-carbon electrode, a platinum wire counter electrode and a silver wire as quasi reference electrode. During the LSV measurement of **1** and **2** a formation of gas bubbles was observed after applying a voltage at the electrodes. The gas formation continued after stopping the LSV measurement until the whole IL turned into a yellow amorphous compound. Analysis of decomposed **2** by ^{1}H NMR spectroscopy showed the formation of a new triplet of quartet signal at $\delta = 6.98$ ppm. ^{19}F NMR spectroscopy reveals two new resonances at $\delta = -85.5$ ppm and -140.0 ppm indicating the formation of gaseous pentafluoroethane during the LSV-measurement. The resonance of the proton at the C2 carbon atom of the imidazolium unit ($\delta = 9.1$ ppm) was greatly reduced, and suggests proton abstraction at this position under formation of pentafluoroethane (see Supporting Information, Figures S9–S10).

During the LSV measurement of the gallate-TAAILs no gas evolution or decomposition was detected. The gallate-TAAILs

Figure 3. Dynamic viscosities of EMIM, BMIM and phenyl TAAIL-gallates.

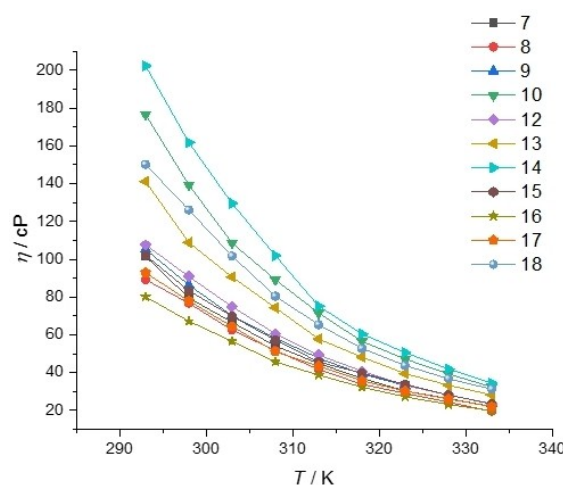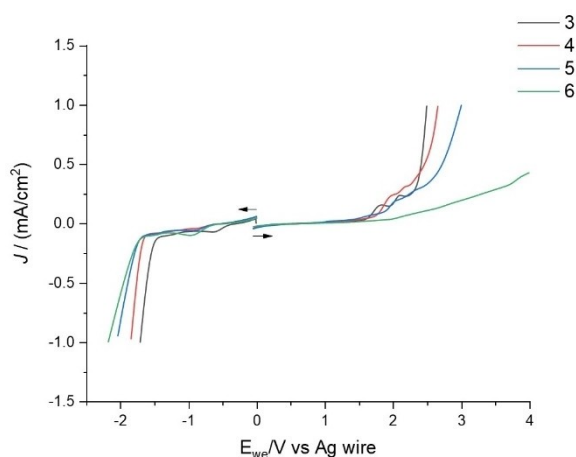| Table 1. Viscosities of 1-ethyl-3-methyl imidazolium salts at 40 °C.	
Anion	η / cP
[B(CF$_3$)$_4$]$^-$	–[a]
[BF$_2$(CN)$_2$]$^-$	7.1[24]
[Ga(C$_2$F$_5$)$_4$]$^-$	19
[NTf$_2$]$^-$	19.4[25]
[Al(OCH(CF$_3$)$_2$)$_4$]$^-$	24.4[15a]
[a] Melting point 125 °C.[26]	

Figure 4. Dynamic viscosities of the 2-Me (**7–10**), 4-OMe (**12–14**) and 2,4-F (**15–18**) substituted TAAIL-gallates.

7–**10** showed a very slow decomposition in a sealed tube, which took place over weeks and turned to a brown highly viscous compound slowly. No decomposition products could be identified by ^1H NMR spectroscopy due to poor solubility and broad resonances. All other gallate-TAAILs showed no decomposition even after several weeks of storage.

The electrochemical window (EW) results from the difference between the cathodic and anodic limits and was determined with a cut-off at ± 0.5 mA/cm^2. Figure 5 shows the LSV measurements of **3**–**6** starting at 0 V. The cathodic and anodic limits increase with chain length with a smaller effect on the cathodic side. The EW increases in the row from **3** (4.02 V) to **4** (4.22 V) to **5** (4.61 V, Figure 5, Table 2). Compound **6** shows a very narrow increase of the current density at high potentials, therefore the cut-off limit was set to 0.2 mA/cm^2. This phenomenon could not be observed in any other gallate-TAAIL and qualifies **6** as a particularly stable ionic liquid at high potentials

with an EW of 4.98 V. The 2-Me substituted gallate-TAAILs **7**–**10** exhibit similar EWs with 4.29 V (**9**) and 4.59 V (**10**). The 2,4-F substituted gallate-TAAILs possess the highest EWs, especially **16** and **18** with values of 4.90 V and 5.15 V, respectively. Table 2 contains the data of the cathodic and anodic limits as well as the electrochemical window for all gallate-TAAILs.

The specific conductivities of the gallate-TAAILs **2**–**10** and **12**–**18** were determined at 25 °C. Again, compounds **1** and **11** were not included due to their relatively high melting point. A linear conductivity decrease is observed for the phenyl substituted compounds and their 2-Me and 2,4-F derivatives in accordance to increasing alkyl chain lengths (Table 2, goodness of fit of $R^2 > 0.98$). The unsubstituted TAAILs exhibit the highest conductivities followed by the 2,4-F and the 2-Me derivatives. The conductivities of the 4-OMe derivatives are overall lower than the other TAAILs and do not decrease linearly with varying alkyl chains. The great potential of the weakly coordinating gallate anion $[Ga(C_2F_5)_4]^-$ is demonstrated by a conductivity increase of 5080 µS in **2** relative to the $[NTf_2]^-$-IL (4017 µS/cm)[30] and the $[BF_4]^-$-IL (3530 µS).[31]

Conclusion

A new type of tunable aryl alkyl ionic liquids (TAAILs) featuring the weakly coordinating anion $[Ga(C_2F_5)_4]^-$ is reported. The viscosities, conductivities and the electrochemical windows were determined for different substituents at the aryl moiety and different alkyl chain lengths. The gallate-TAAILs show an overall low viscosity and large electrochemical windows of up to 5.15 V. For comparison, $[EMIM][Ga(C_2F_5)_4]$ and $[BMIM][Ga(C_2F_5)_4]$ were synthesized leading to ILs with very low viscosities of up to 29 cP at 25 °C. While BMIM- and EMIM-gallate show electrochemical instability, the gallate-TAAILs are stable even up to high potentials.

Figure 5. Linear sweep voltammetry of unsubstituted TAAILs **3**–**6**. Working electrode: glassy carbon (7.07 mm^2); counter electrode: Pt-wire; reference electrode: Ag-wire; scan rate: 50 mV/s.

Experimental Section

Crystal-structure analysis: Deposition Number(s) 2081532 (for **4**) contain(s) the supplementary crystallographic data for this paper. These data are provided free of charge by the joint Cambridge Crystallographic Data Centre and Fachinformationszentrum Karlsruhe Access Structures service www.ccdc.cam.ac.uk/structures.

Conflict of Interest

The authors declare no conflict of interest.

Table 2. Physicochemical data of **2**–**10** and **12**–**18**. Viscosities η and specific conductivity κ were measured at 25 °C. Anodic and cathodic cut-off limit: 0.5 mA/cm^2.

	η / cP	κ/µS/cm	Cathodic Limit/V	Anodic Limit/V	EW/V
2[a]	29	5080	–	–	–
3	70	2141	−1.61	2.41	4.02
4	66	1730	−1.76	2.46	4.22
5	92	979	−1.89	2.72	4.61
6	113	475	−1.95	3.03[b]	4.98
7	80	1615	−1.84	2.52	4.36
8	77	1274	−2.08	2.40	4.48
9	86	778	−1.89	2.40	4.29
10	139	330	−2.01	2.58	4.59
12	91	1057	−1.55	2.02	3.57
13	109	440	−1.68	2.12	3.80
14	162	318	−1.81	2.62	4.43
15	83	1883	−1.56	2.50	4.06
16	67	1373	−2.07	2.83	4.90
17	78	821	−1.91	2.63	4.54
18	126	425	−1.75	3.40	5.15

[a] No CV data due to decomposition, [b] electric density cut-off at 0.2 mA/cm^2.

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