**Introduction**

The electrolyte solution is an important soft material, as well as an electrode solid material, in electrochemical energy storage devices such as lithium-ion batteries (LIBs). In commercial LIBs, organic electrolytes based on carbonate-type solvents [a mixture of cyclic and linear carbonates, such as ethylene carbonate and dimethyl carbonate, respectively] and Li salts (such as LiPF$_6$) are commonly used with a salt concentration of around 1 mol dm$^{-3}$. For most LIBs, the Li salt concentration ($c_{Li}$) has been optimized for ionic conductivity, which is one of the crucial factors for LIB performance. The optimum $c_{Li}$ comes from the maximum ionic conductivity balanced between concentration of ion carriers and viscosity, resulting in $c_{Li} = 1$ mol dm$^{-3}$ in conventional organic electrolytes. Recently, a novel concept for practical LIB electrolyte materials with high-voltage operation has been proposed, i.e., super-concentrated electrolytes. This concept has been widely investigated, not only in the field of LIB chemistry/technology, but also for fundamental science at the molecular level, both experimentally and theoretically. Highly concentrated electrolytes can be successfully applied to both non-aqueous and aqueous solution systems to enable reversible, stable, and working LIBs with adequate electrode materials.

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**Keywords** Salt-concentrated electrolytes, solvation, ion-pair complex, Raman spectroscopy
calculations and MD simulations] study,\textsuperscript{18,28} we proposed that (1) the Li ions are coordinated by both DMF and TFSA in the concentrated region (\(c_{Li} > 2\) mol dm\(^{-3}\)) to form long-range ion-ordering structures based on extended multiple Li-ion complexes, \([\text{Li}^+\cdots\text{TFSA}^–\cdots\text{Li}^+]_n\); and (2) the ion-ordering structure plays a crucial role in the electrochemical stability and the ion-conducting mechanism of the electrolyte, resulting in unique LIB performance for salt-concentrated electrolytes. In the formation of an ion-ordering structure, or multiple-ion-pair complex like \([\text{Li}^+\cdots\text{TFSA}^–\cdots\text{Li}^+]_n\), how the TFSA anion in the salt-concentrated electrolytes coordinates might be essential for controlling and designing the ordering structure and subsequent electrochemical properties; however, knowledge of this process at the molecular level is still, at present, limited.

For TFSA-based ionic liquid electrolytes (\(c_{Li} < 1\) mol dm\(^{-3}\)), TFSA anions have been established to act as a bidentate ligand and bind to the Li ions through two oxygen atoms.\textsuperscript{29–33} Furthermore, we reported that, in an ionic liquid containing the bis(fluorosulfonyl)amide (FSA) anion, which is a molecularly similar anion to TFSA, the Li ions are coordinated with one FSA ligand in a bidentate mode and two FSA ligands in a monodentate mode, forming the \([\text{Li}(\text{FSA})_3]^2–\) complex as an average structure.\textsuperscript{34} Thus, in this work, we focus on the anion coordination behavior of the ion-pair complexes formed in salt-concentrated aqueous electrolytes; particularly, the \(c_{Li}\) dependence of the TFSA coordination types (monodentate, bidentate ligands, or other). The structures of Li-ion complexes were investigated in aqueous LiTFSA electrolytes over a wide \(c_{Li}\) range, up to 5.2 mol dm\(^{-3}\), via IR spectroscopy with the aid of DFT calculations, ionic conductivity measurements, and viscosity measurements.

**Experimental**

**Materials**

LiTFSA salt (Kanto Chemical, battery grade) was used after vacuum drying at 373 K for 100 h. Sample solutions were prepared by dissolving the dried LiTFSA in deionized water to the required molarities (\(c_{Li}\)). The \(c_{Li}\), mole fraction (\(x_{Li}\)), and density (\(d\)) values of the aqueous LiTFSA solutions examined herein are listed in Table S1 (Supporting Information).

**Raman spectroscopy**

Raman spectroscopy was carried out using a dispersion Raman spectrometer (Jasco, NRS-3100) equipped with an argon ion laser at room temperature. The Raman spectra were measured with a laser power of 10 mW at 532.2 nm. The Raman spectra obtained were analyzed using a nonlinear least-squares curve fitting to extract single bands. The detailed analysis procedure is described in our previous work.\textsuperscript{35,36} The integrated intensities of the single bands for the free TFSA in the bulk that was not coordinating Li ion (termed free TFSA) and TFSA bound to Li ion (termed bound TFSA) were represented as \(I_f = J_f \cdot c_f\) and \(I_b = J_b \cdot c_b\), where \(J_f\) and \(J_b\) are the Raman scattering coefficient and \(c_f\) and \(c_b\) are the concentrations of free and bound components, respectively.

**Ionic conductivity and viscosity**

The ionic conductivity was measured by the alternating current impedance method in the frequency range from 100 kHz to 10 mHz using a frequency response analyzer (Solartron, SI-1260). A cell with platinum electrodes was used for the measurements. The cell constant was determined using aqueous KCl solutions (0.01, 0.1, and 1.0 mol dm\(^{-3}\)). The viscosity was measured using a rotating cone-shaped disc-type viscometer (Brookfield, DV-I prime viscometer). Both ionic conductivity and viscosity measurements were conducted at 298 K.

**DFT calculations**

DFT calculations were conducted using the Gaussian 09 software package.\textsuperscript{37} The geometries of isolated TFSA (\(cis\) conformer)\textsuperscript{38,39} and Li-ion complexes were fully optimized at the B3LYP/6-311G** level, followed by normal frequency analyses.

**Results and Discussion**

Figure 1(a) shows the Raman spectra (700 - 790 cm\(^{-1}\) region) for aqueous LiTFSA solutions of various \(c_{Li}\). In the lower \(c_{Li}\) solutions (\(<3.0\) mol dm\(^{-3}\)), the peak observed at 745.2 cm\(^{-1}\) was assigned to the CF\(_3\) bending vibration coupled with the S-N-S symmetric stretching vibration \([\delta(CF_3) + \nu(SNS)]\) of the TFSA anion in the bulk (i.e., free TFSA).\textsuperscript{38} The peak linearly increased in intensity with increasing \(c_{Li}\) up to 3.0 mol dm\(^{-3}\) and the peak
position remained unchanged. This suggested that no coordination of TFSA anions to Li ions occurs at lower $c_{\text{Li}}$; that is, the Li ions are solvated entirely by solvent H$_2$O molecules to form [Li(H$_2$O)$_4$]$^+$ clusters and no contact ion-pairs, like Li$^+$$\cdots$TFSA$^-$, are present. Further increasing $c_{\text{Li}}$ over 3.0 mol dm$^{-3}$ leads to a gradual shift in the peak position to higher frequencies, as highlighted by the solid red lines in Fig. 1(a). Figure 1(b) shows the peak position plotted against $c_{\text{Li}}$, indicating that the peak shifting begins near 3.0 mol dm$^{-3}$ and reaches 749.0 cm$^{-1}$ at maximum $c_{\text{Li}}$ examined (5.2 mol dm$^{-3}$).

A similar behavior was also observed for the S=O vibration peak of the TFSA anion in the 1110 – 1160 cm$^{-1}$ frequency window (Figs. S1(a) and S1(b) in Supporting Information). The peak shifting suggests that the TFSA anions coordinate with Li ions and form ion-pair complexes starting near 3.0 mol dm$^{-3}$. To discuss the $c_{\text{Li}}$ dependence of the structural change in Li-ion solvation and/or contact ion-pair formation in detail, we performed a quantitative curve-fitting deconvolution analysis of the observed Raman spectra to extract the single constituent bands.

Figure 2 shows the typical curve-fitting results for $c_{\text{Li}}$ at (a) 1.0 mol dm$^{-3}$, (b) 3.5 mol dm$^{-3}$, and (c) 5.0 mol dm$^{-3}$ solutions in the 700 – 790 cm$^{-1}$ range. In the dilute solution ($c_{\text{Li}} = 1.0$ mol dm$^{-3}$, Fig. 2(a)), the Raman spectrum could be represented with only one component (745.2 cm$^{-1}$) corresponding to free TFSA, as described above. In the $c_{\text{Li}} = 3.5$ mol dm$^{-3}$ solution (Fig. 2(b)), we found that the spectrum could be successfully deconvoluted into two component peaks at 745.2 and 748.4 cm$^{-1}$; one corresponds to free TFSA and the other to a bound TFSA species. Here, we note the frequency difference between the free and bound species was small ($\Delta \nu = 3.2$ cm$^{-1}$) compared with the corresponding value ($\Delta \nu = 5 – 6$ cm$^{-1}$) reported for TFSA-based ionic liquid electrolytes containing dissolved LiTFSA.$^{28-33}$ The bound TFSA at 748.4 cm$^{-1}$ might be ascribed to the TFSA bound to one Li ion as a monodentate ligand (mono-TFSA), which will be discussed in detail in the DFT calculations section. In a highly concentrated solution ($c_{\text{Li}} = 5.0$ mol dm$^{-3}$, Fig. 2(c)), the peak was deconvoluted into three components (745.2, 748.4, and 751.0 cm$^{-1}$), corresponding to one free and two bound TFSA components. This result implied that the bound mono-TFSA anion (748.4 cm$^{-1}$) coexists with the other type of bound TFSA in the Li-ion coordination sphere. We believe the 751.0 cm$^{-1}$ band to originate from bi-TFSA and/or TFSA in multiple ion-pair complexes (aggregates), as will be discussed in detail later. To obtain more insight into the band-assignment discussed above, we performed DFT calculations on the free and bound TFSA species. Figure 3 shows the theoretical Raman bands for isolated TFSA (as a model of “free TFSA”), the [Li(TFSA)(H$_2$O)$_3$] complex with mono-TFSA, and the [Li(TFSA)(H$_2$O)$_2$] complex with bi-TFSA calculated by DFT calculations, together with the observed Raman bands for the $c_{\text{Li}} = 5.0$ mol dm$^{-3}$ solution. We found that the theoretical band corresponding to the TFSA [$\delta$(CF$_3$) + $\nu$(SNS)] vibration shifted to the higher frequency side in the following order: free TFSA < mono-TFSA < bi-TFSA. This trend was also found in the theoretical bands from the coordination complexes after correcting for a secondary hydration sphere of Li ions, i.e., Li(TFSA)(H$_2$O)$_{\text{mono}}$→(H$_2$O)$_{\text{agg}}$ (see Fig. S2, Supporting Information). The DFT calculations herein are consistent with the experimental results shown in Fig. 3(a); thus, we concluded that the experimental Raman band at around 748.4 cm$^{-1}$ could be assigned to the mono-TFSA species and that the band at 751.0 cm$^{-1}$ could be assigned to the bi-TFSA (or aggregate TFSA) species. Indeed, the similar observation: i.e., free TFSA < mono-TFSA < bi-TFSA in the frequency position, was reported in the ionic liquid electrolyte system using Raman spectra and DFT calculations.$^{36}$

Figure 4 shows the fraction of TFSA species [free TFSA, mono-TFSA, and bi-TFSA (or aggregate TFSA)] to total TFSA ($c_{\text{Li}}$: $c_{\text{f}}$/$c_{\text{Li}}$, $c_{\text{mono}}$/$c_{\text{Li}}$, and $c_{\text{bi/agg}}$/$c_{\text{Li}}$, respectively. The $c_{\text{f}}$, $c_{\text{mono}}$ and $c_{\text{bi/agg}}$ plotted against $c_{\text{Li}}$ are also shown in Fig. S3 (Supporting Information). The detailed procedure is described in Supporting Information. In the lower concentration region (<3.0 mol dm$^{-3}$), TFSA$^-$ anions only exist as free TFSA in the bulk; thus, Li$^+$ ions exist as the hydrated complex, [Li(H$_2$O)$_4$]$^+$.
The fraction of free TFSA remained unchanged up to $c_{Li} \approx 3.0$ mol dm$^{-3}$ and began to decrease linearly with increasing $c_{Li}$, followed by the increase in the fraction of mono-TFSA. This indicated that the free TFSA anions coexist with the mono-TFSA species in the coordination sphere of Li ions in the 3.0 – 4.0 mol dm$^{-3}$ $c_{Li}$ region. The bi-TFSA appeared at $c_{Li} \approx 4.2$ mol dm$^{-3}$ and then gradually increased with increasing $c_{Li}$. Thus, it is plausible that in the concentrated region ($c_{Li} > 4.0$ mol dm$^{-3}$), various types of intricate Li-ion complexes, including H$_2$O, mono-TFSA, and bi-TFSA, coexist simultaneously.

Figure 5 shows the Raman spectra in the range 2800 – 4000 cm$^{-1}$ for aqueous LiTFSA solutions. The two broad peaks at 3255.5 and 3403.0 cm$^{-1}$ monotonically decreased with increasing $c_{Li}$, indicating that the hydrogen bonding network in the bulk gradually ruptured with additional Li salt. At the highest $c_{Li}$ examined here, the hydrogen bonding network disappears completely. Instead, a new peak was found at 3562.5 cm$^{-1}$ that increased in intensity with increasing $c_{Li}$, which might be ascribed to water molecules bound to Li ions.

Figure 6 shows the $c_{Li}$ dependence of the Walden plots for the aqueous LiTFSA solutions obtained from both their molar conductivity ($\Lambda$) and viscosity ($\eta$) at 298 K. It is well known that a plot based on the Walden rule$^{43}$ (i.e., $\Lambda \eta = $ constant) is useful for discussing the dissociativity of a salt in an electrolyte solution; that is, the vertical deviation of the experimental plot from an ideal line (aqueous KCl solution) is one good measure for predicting the extent of salt dissociation and/or ion pairing.$^{44,45}$ From Fig. 6, the Walden plot was located close to the ideal KCl line in the $c_{Li}$ range (1.0 to 3.0 mol dm$^{-3}$). This corresponded well with plots from our previous work on typical organic electrolyte systems containing LiTFSA salt.$^{28,36,45}$ The distance between the experimental plot and the ideal line did not change significantly, even while increasing the $c_{Li}$ up to 3.0 mol dm$^{-3}$. In the highly concentrated solutions ($c_{Li} > 3.0$ mol dm$^{-3}$) according to the Raman and DFT results in this work, Li ions directly interacted with TFSA anions to form Li$^+ \cdots$TFSA$^-$ contact ion-pair complexes; i.e., the dissociativity of the LiTFSA salt was significantly low. However, further increasing $c_{Li}$ over 3.0 mol dm$^{-3}$ caused the Walden plot to resemble the ideal line even more closely (Fig. 6). This result implied that the ion-conducting mechanism considerably changes in a highly salt-concentrated region from the dilute region; i.e., the Grothuss mechanism (or Li-ion hopping in this case) might be dominant in concentrated solutions, an alternative to the vehicle mechanism in dilute solutions. In a dilute system, it is well known that a plot based on the Walden rule$^{41}$ (i.e., $\Lambda \eta = $ constant) is useful for discussing the dissociativity of a salt in an electrolyte solution; that is, the vertical deviation of the experimental plot from an ideal line (aqueous KCl solution) is one good measure for predicting the extent of salt dissociation and/or ion pairing.$^{44,45}$ From Fig. 6, the Walden plot was located close to the ideal KCl line in the $c_{Li}$ range (1.0 to 3.0 mol dm$^{-3}$). This corresponded well with plots from our previous work on typical organic electrolyte systems containing LiTFSA salt.$^{28,36,45}$ The distance between the experimental plot and the ideal line did not change significantly, even while increasing the $c_{Li}$ up to 3.0 mol dm$^{-3}$. In the highly concentrated solutions ($c_{Li} > 3.0$ mol dm$^{-3}$) according to the Raman and DFT results in this work, Li ions directly interacted with TFSA anions to form Li$^+ \cdots$TFSA$^-$ contact ion-pair complexes; i.e., the dissociativity of the LiTFSA salt was significantly low. However, further increasing $c_{Li}$ over 3.0 mol dm$^{-3}$ caused the Walden plot to resemble the ideal line even more closely (Fig. 6). This result implied that the ion-conducting mechanism considerably changes in a highly salt-concentrated region from the dilute region; i.e., the Grothuss mechanism (or Li-ion hopping in this case) might be dominant in concentrated solutions, an alternative to the vehicle mechanism in dilute solutions. In a dilute system, it is well known that the dominant ion diffusion (solvated Li ions and anions without ion pairing) is based on the Stokes-Einstein law. In the current aqueous LiTFSA solutions, we demonstrated using Raman spectroscopy that no contact ion pairs formed between Li ions and TFSA anions below $c_{Li} = 2$ – 3 mol dm$^{-3}$. To a highly concentrated LiTFSA solution ($c_{Li} > 3.0$ mol dm$^{-3}$), most of the Li ions are directly coordinated with the TFSA anions to form contact ion pairs as the major

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**Fig. 4** Fraction of the TFSA species in aqueous LiTFSA solutions: free TFSA ($c_f/c_{Li}$, black), bound mono-TFSA ($c_{b(mono)}/c_{Li}$, red), and bound bi-TFSA or aggregate TFSA ($c_{b(bi/agg)}/c_{Li}$, blue).

**Fig. 5** Raman spectra in the range 2800 - 4000 cm$^{-1}$ observed for aqueous LiTFSA solutions.

**Fig. 6** $c_{Li}$ dependence of Walden plots for aqueous LiTFSA solutions at 298 K.
species. Hence, we expect that the vehicle mechanism cannot be applied for understanding the ion-conducting behavior in a highly concentrated solution with little to no free water molecules in the bulk. Thus, the Grotthuss mechanism is expected to be active in the concentrated electrolyte system. Indeed, recent simulation studies suggested that an extended ion-ordering structure based on a multiple Li-ion complexes formed in a concentrated electrolyte system contribute to the unusual Li-ion transport with the Grotthuss mechanism.3,13,28,46

Conclusions
The TFSA coordination behavior in highly concentrated aqueous electrolyte containing LiTFSAnan salt was characterized structurally using Raman spectroscopy and DFT calculations. Based on a quantitative distribution analysis of the TFSA species and ionic conductivity/viscosity studies, we found the following. (1) In the lower $c_{Li}$ region (below 3.0 mol dm$^{-3}$), no coordination was observed between the TFSA anions and the Li ions. (2) TFSA anions coordinate with Li ions in a monodentate manner in the $c_{Li} = 3.0 - 4.0$ mol dm$^{-3}$ region. (3) Further increasing $c_{Li}$ leads to bidentate-type TFSA (bi-TFSA) bound to Li ion (starting at $c_{Li} = 4.2$ mol dm$^{-3}$) to yield multiple types of intricate (and/or multiple) Li-ion complexes where the ligands can include H$_2$O, mono-TFSA, and bi-TFSA. (4) In the highly concentrated region, Li ions might form an ion-ordering structure based on multiple Li-ion complexes (Li$^+$.·.·TFSA$^-$·.·.·Li$^+$) and the Walden plot closely resembles that of the ideal KCl line. Therefore, a change in the ion-conducting mechanism from the vehicle mechanism to the Grotthuss mechanism likely occurs when $c_{Li}$ exceeds 4.2 mol dm$^{-3}$.

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Supporting Information
This material is available free of charge on the Web at http://www.jsac.or.jp/analsci/

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