Glyme-Li salt equimolar molten solvates with iodide/triiodide redox anions

Keisuke Shigenobu, Azusa Nakanishi, Kazuhide Ueno,* Kaoru Dokko, and Masayoshi Watanabe

Department of Chemistry and Biotechnology, Yokohama National University, 79-5 Tokiwadai, Hodogaya-ku, Yokohama 240-8501, Japan.

CORRESPONDING AUTHOR: To whom correspondence should be addressed. Telephone/Fax: +81-45-339-3951. E-mail: ueno-kazuhide-rc@ynu.ac.jp
Chemical diffusion coefficient of anions and ionicity

The limiting current value (\(I_{\text{lim}}\)) are defined in eq. S1. The chemical diffusion coefficient was obtained by substituting the current value for the following:

\[
|I_{\text{lim}}| = 4nFcDr_0 \quad \text{(S1)}
\]

where \(n\) denotes the number of electrons, \(F\) for Faraday constant, \(c\) for concentration of an anion, \(D\) for chemical diffusion coefficient and \(r_0\) for disk electrode radius.

The molar conductivity ratio (ionicity, \(\Lambda/\Lambda_{\text{NE}}\)) was calculated by dividing the ideal ionic conductivity (\(\Lambda_{\text{NE}}\)) into the experimental one (\(\Lambda\)). Finally, these values are summarised in Table S1.

Table S1 Diffusion coefficients, molar conductivities and ionicity of [Li(G4Et)]I and [Li(G4Et)]I₃ at 60 °C.

| Sample       | \(D_G\) \([\times 10^{-7} \text{ cm}^2\text{s}^{-1}]\) | \(D_{Li}\) \([\times 10^{-7} \text{ cm}^2\text{s}^{-1}]\) | \(D_{\text{anion}}\) \([\times 10^{-7} \text{ cm}^2\text{s}^{-1}]\) | \(\Lambda\) \([\text{S cm}^2\text{mol}^{-1}]\) | \(\Lambda_{\text{NE}}\) \([\text{S cm}^2\text{mol}^{-1}]\) | \(\Lambda/\Lambda_{\text{NE}}\) |
|--------------|---------------------------------|---------------------------------|---------------------------------|----------------|---------------------------------|----------------|
| [Li(G4Et)]I   | 0.86                            | 0.76                            | 4.36                            | 0.46           | 1.73                            | 0.27            |
| [Li(G4Et)]I₃  | 4.46                            | 4.87                            | 2.84                            | 2.89           | 2.61                            | 1.11            |
Theoretical gravimetric capacity of catholyte.

Theoretical gravimetric capacity of catholyte ($C_C$) is given below:

$$C_C \text{[mAh g}^{-1}] = 100nF/3600M_C \quad (S2),$$

where $n$ indicates the number of moles relating to electron transfer, $M_C$ for the total molecular weight of catholyte and $F$ for Faraday constant. Thus, the capacity of $[\text{Li(}\text{G}4\text{Et})\text{I}]_3$ was calculated to 85.91 mAh g$^{-1}$.

![Fig. S2 Time-dependent cell voltage of [Li(G4Et)]I and [Li(G4Et)]I$_3$.](image)

![Fig. S3 DSC curve of [Li(G4Et)$_{1/3}$]I.](image)
Fig. S4 (a) Charge-discharge curves of Li | 1 mol dm$^{-3}$ Li[TFSA] in G4Et | LIGC | 1 mol dm$^{-3}$ LiI$_3$ in G4Et cell at 60 °C. (b) charge-discharge capacity and Coulombic efficiency as a function of cycle number.