Supporting Information for: Complete Characterization of a Lithium Battery Electrolyte using a Combination of Electrophoretic NMR and Electrochemical Methods

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1. Salt Concentration Determination for LiTFSI/tetraglyme Electrolytes

Concentrations of the electrolytes used in this work are given in Table S1, showing the conversion between \( r \), corresponding to the ratio of lithium ions to ether oxygens in tetraglyme (\( r = ([\text{Li}^+] / [\text{O}]) \)) and molality, \( m \), or moles of LiTFSI salt per kilogram of tetraglyme.

\begin{table}[h]
\centering
\begin{tabular}{|c|c|}
\hline
\( r \) ([\text{Li}^+] / [\text{O}] ) & \( m \) (mol/kg) \\
\hline
0.008 & 0.18 \\
0.016 & 0.36 \\
0.032 & 0.72 \\
0.048 & 1.08 \\
0.064 & 1.45 \\
0.08 & 1.79 \\
0.096 & 2.16 \\
0.112 & 2.52 \\
\hline
\end{tabular}
\caption{Salt concentration equivalencies for LiTFSI/tetraglyme electrolytes}
\end{table}

2. Diffusion Coefficient Fitting
3. Error determination

This section of the SI details equations used to determine error for all of the derived parameters in this work. Error formulas are based on standard error propagation. Error for measured parameters is based on standard deviation of multiple measurements.

\[ \frac{dU}{d\ln m} \]

Formula for determining error in \( \frac{dU}{d\ln m} \) based on the finite difference method, where \( x_1 \) and \( y_1 \) refer to the ln(molality) and OCV, respectively, for the first data point:

\[
\delta \left( \frac{y_3 - y_1}{x_3 - x_1} \right) = \left| \frac{y_3 - y_1}{x_3 - x_1} \right| \sqrt{\left( \frac{\delta y_3}{y_3 - y_1} \right)^2 + \left( \frac{\delta y_1}{y_3 - y_1} \right)^2}
\]

(S3.1)

Error formula for thermodynamic factor based on electrochemical methods, \( T_{f,\text{echem}} \):

\[
\delta \left( 1 + \frac{dlny \pm dln m}{dln m} \right) = \left| 1 + \frac{dlny \pm dln m}{dln m} \right| \sqrt{\left( \frac{\delta k}{k} \right)^2 + \left( \frac{\delta D}{D} \right)^2 + \left( \frac{\delta \rho}{\rho} \right)^2 \rho^2 + 2 \left( \left( \frac{\delta dU}{dlnm} \right)^2 \right)^2}
\]

(S3.2)

Error formula for the transference number based on electrochemical methods, \( t_{+ \text{,echem}}^0 \):

\[
\delta t_{+}^0 = \left| t_{-}^0 \right| \sqrt{\left( \frac{\delta k}{k} \right)^2 + \left( \frac{\delta D}{D} \right)^2 + \left( \frac{\delta \rho}{\rho} \right)^2 + \left( \frac{\delta dU}{dlnm} \right)^2}
\]

(S3.3)
Error formula for calculation of the thermodynamic factor using eNMR and concentration cells, $T_{f, eNMR}$:

$$
\delta \left( 1 + \frac{d\ln y}{d\ln m} \right) = \left| 1 + \frac{d\ln y}{d\ln m} \right| \sqrt{\left( \frac{\delta t_0}{t_0}\right)^2 + \left( \frac{\delta U}{dU/d\ln m} \right)^2}
$$

(S3.4)