

## Important factors for the reliable and reproducible preparation of non-aqueous electrolyte solutions for lithium batteries

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Electrolyte solutions play a crucial role in rechargeable lithium batteries. Driven by an ever-increasing demand for better batteries, more and more stringent performance requirements are being asked of electrolytes. This demand to achieve electrolytes beyond the state-of-the-art has driven an increasing number of publications over the past decade. Nevertheless, a detailed description of electrolyte preparation is frequently missing when reporting new electrolytes for batteries, creating a barrier for others to reproduce important findings. In addition, false or misleading information in a paper may result from unintentional inaccuracies during the electrolyte preparation process. This article highlights important factors for the reliable and reproducible preparation of non-aqueous electrolyte solutions for lithium batteries, with the aim of encouraging researchers to follow more rigorous reporting standards.

Lithium (Li) batteries, a technology that ushered in a revolution in energy storage and won the 2019 Nobel Prize in Chemistry, have experienced rapid development over the last decades<sup>1,2</sup>. Based on the success of Li ion batteries (LIBs) and the ever-increasing demand for batteries with improved performance (e.g., high energy/power density, fast charge capability, long cycling/calendaring life and low cost), intensive research efforts have been dedicated to the study of new battery chemistries and materials<sup>3</sup>. In recent years, an electrolyte, which is short for an electrolyte solution in the battery field and colloquially refers to all electrolyte solution components, has been increasingly recognized as important as electrode materials<sup>4</sup>. While electrode materials determine the energy output, the interfacial reactions between electrodes and electrolytes are extremely sensitive to the electrolyte<sup>5–7</sup>.

In many situations, a solid electrolyte interphase (SEI) or cathode electrolyte interphase (CEI), which is derived from the chemical and electrochemical decompositions of electrolyte, has the rate-limiting kinetics that control the rate of mass flow within the battery cell and determines the reversibility of the cathode/anode by changing the side reactions<sup>6,8</sup>. To exploit the full potential of advanced electrode materials, an electrolyte and its associated SEI/CEI must be tailored to specific applications, such as improving the electrolyte's anodic stability for high-voltage cathodes<sup>9</sup>, enhancing Li stability for Li metal batteries (LMBs)<sup>10</sup>, suppressing the solubility of polysulfide for sulfur cathodes<sup>11</sup>, etc. A wealth of publications on electrolytes have therefore been merged into the energy storage field<sup>10,12</sup>. However, a detailed description about electrolyte components and/or a rigorous statement regarding the electrolyte preparation process are still frequently missing, such as a lack of information about supplier, purity, impurities, dryness of the starting chemicals, mixing order of the solutions, appearance of the as-prepared electrolyte, container material, temperature and atmosphere being used for electrolyte storage, and other certain precautions for some specific electrolyte systems. These limitations raise the barrier to ensuring some interesting findings are reproducible by others. In addition, false or misleading

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information may result from unintentional inaccuracies during the electrolyte preparation process. Therefore, descriptions of electrolyte preparation that are oversimplified to the point that basic information is obscured, are not suitable for real applications and publications.

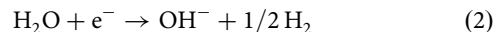
Recently, several journals (*Joule*, *ACS Energy Letters*, and *Journal of Power Sources*) initiated standard checklists for rigorous reporting of battery chemistries to minimize potential misrepresentation and misunderstanding of battery performance<sup>13–15</sup>. These checklists share similar criteria in reporting, including cell type and configuration, electrode type, electrode areal capacity loading (lithium inventory/thickness for LMBs), anode/cathode capacity (N/P) ratio and electrolyte amount (electrolyte/capacity [E/C] ratio).

To achieve reliable publication of electrolyte results and reproducible electrolyte preparation, this article summarizes several important factors affecting the electrolyte quality and puts forward corresponding control measures for electrolyte preparation and standardized reporting.

**Moisture control.** Moisture content is one of the most important factors governing electrolyte quality even trace water in the electrolyte could lead to significant performance variations in the batteries<sup>16–20</sup>. Moisture triggers undesired chemical and electrochemical side reactions in the battery (as shown in Fig. 1a) and accelerates cell decay by degrading the cathode, the anode, and the electrolyte itself. For instance, LiPF<sub>6</sub> hydrolysis is one of the biggest concerns because it leads to production of lithium fluoride (LiF), phosphoryl fluoride (POF<sub>3</sub>), and hydrogen fluoride (HF) (Eq. 1)<sup>18,21–25</sup>.



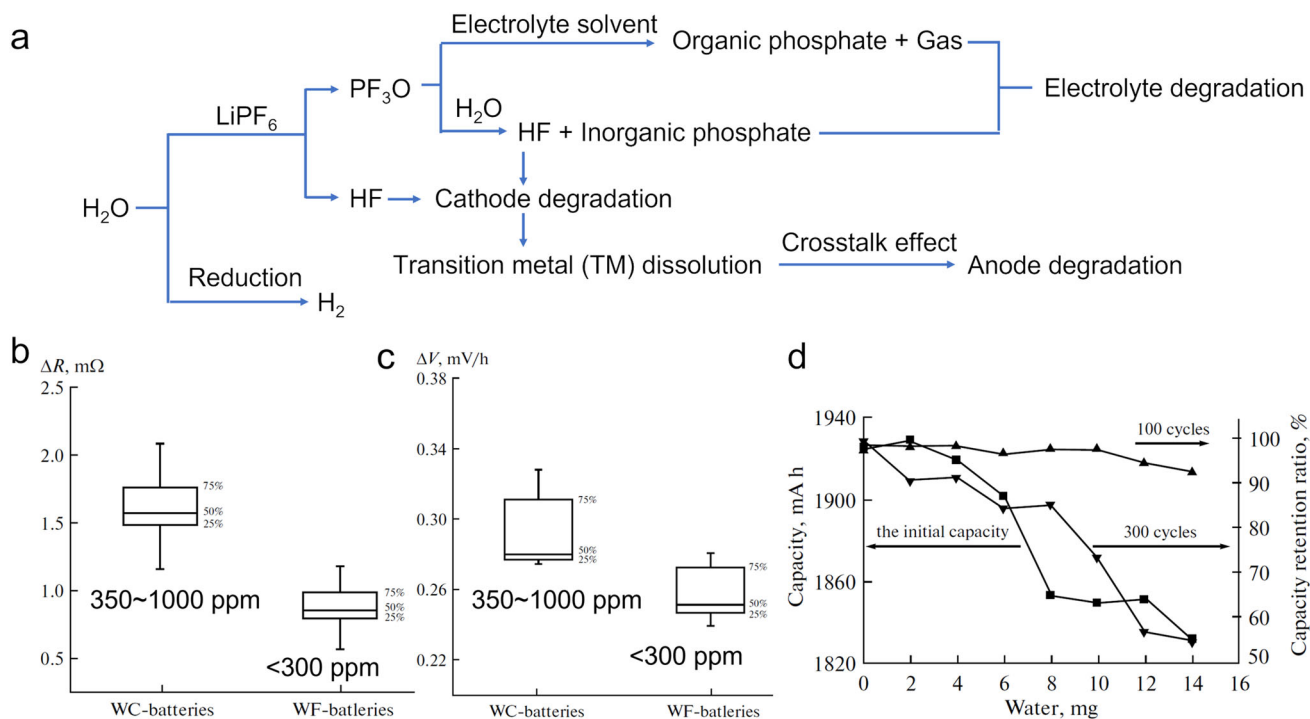
Although the LiF generated by LiPF<sub>6</sub> hydrolysis plays a positive role in the SEI in a few studies<sup>26</sup>, the HF usually has an overwhelming negative role due to its highly corrosive nature, which initiates transitional metal (TM) dissolution from the cathode material and results in cathode degradation<sup>25</sup>. In addition, the TM ions could migrate from the cathode to the anode through the electrolyte and poison the anode.<sup>27</sup> The POF<sub>3</sub> from LiPF<sub>6</sub> hydrolysis may also lead to further electrolyte degradation, forming organic and inorganic phosphate products and generating gases<sup>28</sup>. H<sub>2</sub> generation is another frequently occurrence caused by water in the electrolyte through reduction on the anode (Eq. 2).



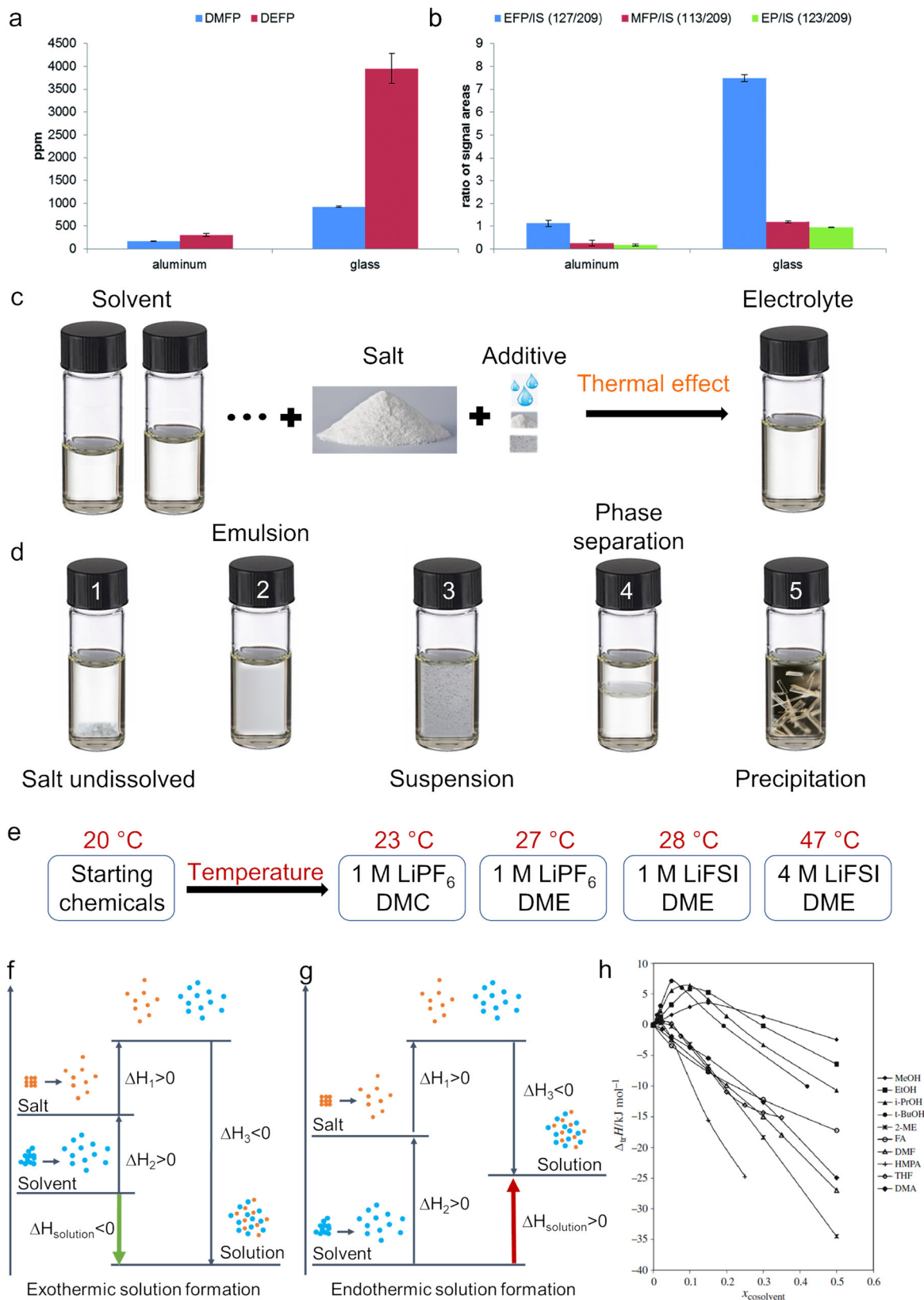
These products as well as the residue H<sub>2</sub>O could affect the performance during battery storage and operation.

For instance, results of a systematic study on the effects of trace H<sub>2</sub>O to 18650-type cylindrical cells (graphite||lithium nickel cobalt manganese oxides [NMC]) are presented in Figs. 1b–d<sup>17</sup>. A water-containing electrolyte leads to increased internal resistance, reduced initial capacity, fast voltage decay during storage, and rapid cycling degradation compared to water-free electrolytes<sup>17</sup>. Therefore, a tight specification for H<sub>2</sub>O content is required to prolong the durability of the batteries. Currently, an empirical and strict water content control of H<sub>2</sub>O < 20 ppm or even 10 ppm is commonly used in the battery industry.

To achieve reliable publishing of electrolyte preparation in the academic field, researchers are encouraged to provide the water content of electrolyte. For novel electrolyte approaches, H<sub>2</sub>O ≤ 20 ppm is recommended to minimize the electrolyte variation caused by water content. Battery-grade anhydrous chemicals



**Fig. 1** Effects of water content on electrolytes. **a** Schematic summary of the effects of water in electrolytes. **b** The internal resistance variation ( $\Delta R$ ) of LIBs before and after charging for water-containing (WC) batteries and water-free (WF) batteries. **c** The voltage variation ( $\Delta V$ ) of LIBs for WC batteries and WF batteries after 168 h aging at a high voltage of 4.2 V. **d** The initial capacities and cycling behaviors (100 cycles and 300 cycles, 0.5 C charging/0.5 C discharging) of batteries contained different water dosages. Reproduced with permission from reference<sup>17</sup>, copyright (Springer Nature, 2014).



(including conducting salts, solvents, and additives) are required for electrolyte preparation, and pre-drying becomes important for hydrous chemicals. Any containers or materials that will be in contact with electrolyte chemicals (such as weighing paper, pipette tips, stirrer, etc.) during the preparation process need to be dried before use to avoid introducing water into the electrolyte.

For research on the effect of water concentration in electrolytes or strategies for relaxing the water specifications of electrolytes<sup>29</sup>, there is no restriction on water content as long as the water content is provided. To achieve this goal, water content determination is essential. The Karl Fischer titration method is highly accurate for trace water detection and is recommended for

**Fig. 2 Container selection and cautions during electrolyte preparation.** Analysis of organic phosphate (dimethyl fluorophosphate [DMFP], diethyl fluorophosphate [DEFP], methyl fluorophosphate [MFP], ethyl fluorophosphate [EFP] and ethylene phosphate [EP]) formation through (a) GC-MS and (b) IC-ESI-MS in 10 mL aluminum and glass vials after aging at 85 °C for 5 days (the GC-MS values of the electrolyte samples stored in glass vials are divided because of the better clarity provide using a factor of 10). Reproduced with permission from reference<sup>41</sup>, copyright (Royal Society of Chemistry, 2015). c Schematic for electrolyte preparation. d Five common mixtures that are less than desirable. e Maximum temperatures detected during 1 mL electrolyte preparation in 7 mL WHEATON® LDPE round bottles, with an environmental temperature of 20 °C. Schematic drawing of the (f) exothermic and (g) endothermic solution formation. h Enthalpies of transfer of NaI from water to water-cosolvent mixtures at 298.15 K. Reproduced with permission from reference<sup>45</sup>, copyright (Springer Nature, 2012).

water content determination and reporting<sup>30</sup>. In addition, the associated HF content, which can be determined using <sup>19</sup>F nuclear magnetic resonance (NMR) or a F-ion selective probe, is also suggested for publication<sup>31</sup>.

**Purity control.** In addition to water, the presence of trace impurities (residual from the manufacturing process of the salt, and solvent) may also profoundly affect the battery performance<sup>32–34</sup>. This issue is of major importance for scientists and engineers in the field. Although a huge variety of potential impurities and related side reactions exist in diversified electrolyte systems, the most unfavorable reactions mainly fall into the following categories. (1) Reactions with salts: protic impurities like alcohols and acids, which are frequently residual from electrolyte solvent manufacturing, react with LiPF<sub>6</sub> and lead to formation of HF (like the reaction between LiPF<sub>6</sub> and water) and greatly affect the electrolyte quality<sup>32</sup>. (2) Electrochemical reactions on electrodes—reduction/oxidation takes place when an unknown impurity has poor reductive/oxidative stability on the anode/cathode, resulting in gas generation and SEI/CEI formation<sup>34</sup>. As mentioned previously, battery performance is highly sensitive to the quality of SEI and CEI due to the interfacial electrochemical reactions of the batteries<sup>6</sup>. In many publications, SEI/CEI additives, even with low concentrations of 1%, 0.5%, and 0.1%, can significantly change the cell performance<sup>35,36</sup>. Therefore, an impurity behaves like an SEI or CEI additive and could significantly change the chemistry, structure, and kinetics of the SEI/CEI. Metal ion residues in the electrolyte are also an example of these impurities, which can be reduced on the anode side and poison the SEI. (3) Chemical reactions with electrodes: electrode corrosion initiates when an impurity reacts with an electrode component. Especially in the LMBs that use Li metal as the anode, Li corrosion by impurities (such as organic acids, alcohols, aldehydes, ketones, amines, and nitriles)<sup>37</sup> could be a big concern due to the highly reactive nature of the metallic Li<sup>38</sup>. As a consequence, the reversibility of the cathode/anode could be considerably changed by such impurities.

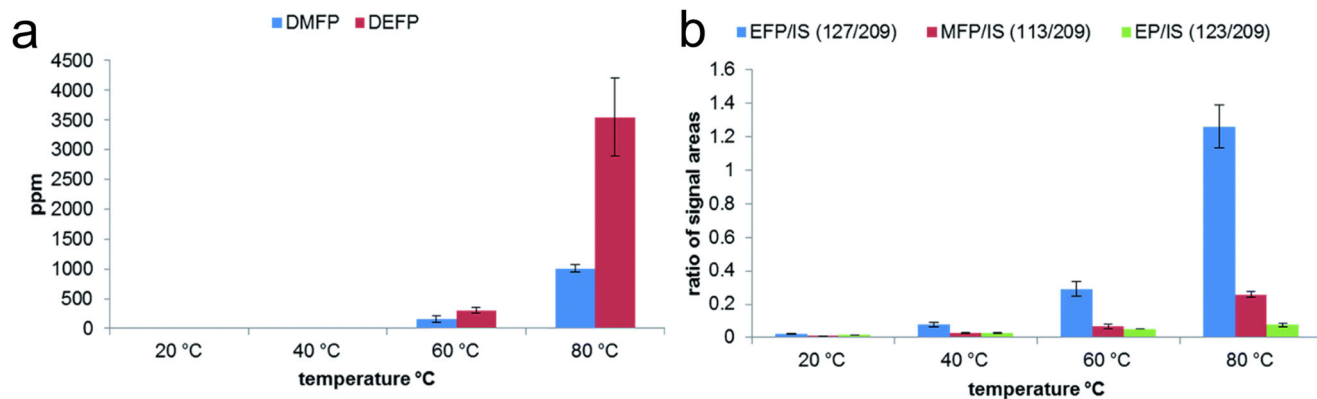
To minimize the potential for irreproducible results from different researchers, purity control of chemicals plays a crucial role in electrolyte preparation. The purity of the chemicals (together with the supplier/vendor information) is required in the publications and impurity identification and chemical purification are also important. Analytical techniques, such as <sup>1</sup>H, <sup>13</sup>C, and <sup>19</sup>F NMR, high-performance liquid chromatography, gas chromatography–mass spectrometry (GC-MS), and ion chromatography with mass spectrometry (IC-MS), are suitable for identifying impurities in most of the chemicals used in the electrolytes<sup>39</sup>. Common methods, including distillation, crystallization, extraction, chromatography, electrophoresis, and etc., can be applied for further purification depending on the physicochemical properties of the chemical and impurities<sup>40</sup>. Frankly speaking, it is impractical to draw a fixed line for purity because of the complexity of battery chemistry and the potential variety of impurities. However, to draw the attention of researchers to the importance of chemical purity and to minimize differences

between research approaches, battery degree purity or a purity above 99% (the higher, the better) are recommended empirically.

**Container selection.** Container selection is also important for electrolyte preparation. In the study by Winter, M. et al., containers made from different materials have distinct effects on electrolyte thermal decomposition<sup>41</sup>. A glass container accelerates LiPF<sub>6</sub> degradation, resulting in more non-ionic (dimethyl fluorophosphate [DMFP] and diethyl fluorophosphate [DEFP], Fig. 2a) and ionic (methyl fluorophosphate [MFP], ethyl fluorophosphate [EFP], and ethylene phosphate [EP], Fig. 2b) organic phosphate accumulation in a classical electrolyte of 1 M LiPF<sub>6</sub> in ethylene carbonate (EC)/ethyl methyl carbonate (EMC) (50/50 wt.%). Only 0.43 M LiPF<sub>6</sub> remains after 5 days of aging at 85 °C in the glass container<sup>41</sup>. The main reason behind this is the reactions between the LiPF<sub>6</sub> hydrolysis product HF and the glass materials (e.g., borax, SiO<sub>2</sub>), which produce water that can further accelerate LiPF<sub>6</sub> degradation<sup>41</sup>. To avoid this, the container must be inert to all the chemicals that are stored in it, and materials like polypropylene (PP), polyethylene (PE), or Al can be suitable for electrolyte containers<sup>41</sup>. It is also worth pointing out that the containers must be airtight to avoid any contamination from the ambient atmosphere, and lighttight containers are suitable for those electrolytes that contain light-sensitive compounds.

**Electrolyte and temperature monitoring during preparation.** In chemistry, a nonaqueous electrolyte is a special type of solution, in which the conducting salt(s) (and functional additives) is(are) dissolved in the organic solvent(s)<sup>5,35</sup>. Upon dissolving, these salt(s) and additive(s) disperse uniformly through the solvent(s), forming a homogeneous electrolyte mixture as shown in Fig. 2c. Because the effects of chemical polarity are involved in the mixing process, unideal mixtures besides the solution form in certain cases as shown in Fig. 2d, including: (1) undissolved conducting salt(s)/additive(s) residue(s), (2) emulsion, (3) suspension, or (4) phase separation of the starting materials, and (5) salt precipitation/recrystallization in an over-saturated solution after resting. Careless slips in checking the solution status could lead to failed electrolyte preparation.

Close attention to thermal effects during the mixing process is important as well. As an example, Fig. 2e records the maximum temperatures detected during 1 mL electrolyte preparation for four single-salt (LiPF<sub>6</sub> or LiFSI), single-solvent (DMC or DME) electrolytes in a 7 mL WHEATON® LDPE round bottle. The temperature measurements started at the beginning of the mixing process (with 20 °C as the environmental temperature) and ended once the salt was fully dissolved. Very different maximum temperatures were detected by varying the solvents, salts and salt concentrations. A maximum temperature of 23 °C was detected in the preparation of 1 M LiPF<sub>6</sub> in DMC, changing to 27 °C with 1 M LiPF<sub>6</sub> in DME, 28 °C in 1 M LiFSI in DME, and 47 °C in 4 M LiFSI in DME. This temperature increase is caused by the heat released during solvation.



**Fig. 3 Storage performance of electrolytes at different temperatures.** Analysis of the organic phosphate (dimethyl fluorophosphate [DMFP], diethyl fluorophosphate [DEFP], methyl fluorophosphate [MFP], ethyl fluorophosphate [EFP] and ethylene phosphate [EP]) formation by (a) GC-MS and (b) IC-ESI-MS in 10 mL aluminum vials after aging at different temperatures for 21 days. Reproduced with permission from reference<sup>41</sup>, copyright (Royal Society of Chemistry, 2015).

As shown in Fig. 2f and g, solvation can either be endothermic or exothermic, where heat is initially absorbed during the bonds breaking in the origin salt(s) (electrostatic attraction between two ions) and solvent(s) (intermolecular attractions between solvent molecules) and released in the formation of new ion-solvent attractive bonds<sup>42</sup>. The overall heat of solvation is the difference between the relative heat required for bond breaking and the heat released during reformation<sup>42</sup>. Few studies have reported the results of calorimetric investigations during electrolyte preparation for Li batteries. However, there is a long history of studying the thermochemistry of solution mixings, especially for water solutions<sup>43–45</sup>. Fig. 2h, as an example, presents the influence of the solvent on the solvation of NaI. Different solvents lead to different enthalpies of NaI solvation. In addition to the total heat from solvation, the highest temperature during electrolyte preparation can also be influenced by many other factors, such as dissolution rate, electrolyte amount, and container material and size/shape, which affects the heat dissipation.

High temperatures during the electrolyte preparation process may affect the salt solubility, resulting in over-saturated electrolytes that cause salt precipitation when the temperature falls back to room temperature<sup>46</sup>. Elevated temperatures may also accelerate electrolyte evaporation and degradation<sup>41</sup>. Therefore, monitoring the temperature during electrolyte preparation is important, particularly when preparing a large quantity of electrolyte for which the heat dissipation is relatively slow. For a mixing process that releases a significant amount of heat, the solvation process can be divided into multiple steps by adding the salt to the solvent gradually until the salt is completely dissolved under a controlled temperature.

**Electrolyte storage.** Electrolyte storage is a follow-on to electrolyte preparation. The ambient environment, including humidity, light, container type, and temperature, are critical for electrolyte storage. As discussed in the previous sections, improper containers, high water content, and light can accelerate electrolyte deterioration. The results in Fig. 3a, b show rapid electrolyte degradation at elevated temperatures. A large amount of LiPF<sub>6</sub> and solvent decomposition products accumulate at temperatures of 60 and 80 °C compared to 20 and 40 °C<sup>41</sup>. Therefore, to obtain reliable battery performance, it is important to store electrolytes in an electrolyte-friendly environment with controlled humidity (such as a glovebox, or dry room) at mild temperatures (no

freezing and no excessive heat) and to use light-tight containers for light-sensitive samples.

While the ambient environment is an external factor that influences electrolyte storage stability, the chemical stability of the electrolyte components also plays a role internally. For instance, fluoroethylene carbonate (FEC), which is a commonly used solvent/additive for conventional electrolytes, can significantly worsen the storage stability of the LiPF<sub>6</sub> carbonate electrolyte due to the interactions between LiPF<sub>6</sub> and FEC that accelerate HF accumulation and trigger electrolyte polymerization<sup>47</sup>. Inspecting the electrolyte quality before use is encouraged, particularly for electrolytes that have been stored for a long time. In an aged electrolyte, decomposition products from the salt, solvent, and additives become additional impurities compared to the as-prepared electrolyte<sup>22,31</sup>. The electrolyte inspection should include but not be limited to water content identification, acid concentration determination, and purity tests using the analysis techniques discussed in the previous sections.

**Outlook.** LIBs will continue as a key technology over the long term because of their omnipresence in consumer electronics, electric vehicles, and electric grids. Due to the market demand for superior performance to meet various applications, increasingly stringent requirements are being imposed on established LIBs, and various exploratory electrochemical systems beyond LIBs are emerging, such as LMBs, sodium batteries, potassium batteries, and zinc batteries. Innovations are critical for developing advanced electrolytes to sustain these desired technological trajectories.

As previously mentioned, slight variations in the electrolyte could lead to widely varied electrochemical performance due to the intrinsic surface-electrochemical nature of the battery charging/discharging processes. Thus, in addition to the checklists launched for cell assembly and reporting<sup>13–15</sup>, it is critical for the community to agree on a set of criteria that can be implemented into electrolyte preparation as well. Table 1 proposes a checklist of experimental details of electrolyte preparation for reporting. Simply publishing an “innovative” electrolyte without providing the quality control information may make the results difficult for others to reproduce and present challenges that inhibit industrial scale-up for practical applications. This checklist could be a beneficial and important when implementing new electrolyte concepts to batteries, which can effectively promote the reliability and reproducibility of the electrolyte in realistic applications.

**Table 1 Recommended checklist in reports for electrolyte preparation.**

	Existing literature	Suggestions
Water content	Checked by limited literature	≤20 ppm
HF content	Checked by limited literature	≤20 ppm
Chemical supplier	Provided by most literature	Provide
Chemical purity	Provided by some literature	≥99%
Impurities	Barely mentioned	Provide if possible
Type of container	Provided by limited literature	Airtight PP, PE, and Al containers, light tight for light-sensitive electrolytes
Electrolyte appearance	Provided by limited literature	Provide color, clarity
Glovebox	Provided by most literature	O <sub>2</sub> ≤ 1 ppm
(O <sub>2</sub> and H <sub>2</sub> O content)		H <sub>2</sub> O ≤ 1 ppm
Dry room	Provided by some literature	Dewpoint ≤ -40 °C
(Dewpoint)		
Storage temperature (T)	Provided by some literature	Freezing point <T < 40 °C

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### Author contributions

X.C. prepared the manuscript.

### Competing interests

The authors declare no competing interests.

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