Description of ‘Electrolyte SMILES’

An example of electrolyte SMILES representation for 1 M LiPF6/EC/EMC/2 wt% VC electrolyte from Chen et al. study (<https://doi.org/10.1016/j.joule.2019.02.004>):

A diagram of a function

Description automatically generated with medium confidence

The electrolyte SMILES will consist of typical SMILES representation for each of the solvent, salt, and additive component species. Each of these components will be separated by ‘>’ sign, similar to how reactants and products are separated in the reaction SMILES. However, there is no option for entering the amount of each component in the reaction SMILES, such as volume, concentration, etc. (extensive variables). For the case of electrolyte SMILES, amount of each specie can be entered within ‘| |’. For example, |0.3v| for EC solvent amount in the above case. The number represents the magnitude, and the following text represents the unit, i.e., v for volume, w for weight, mol for number of moles, M for molarity, m for molality, C for Celsius, K for kelvin, etc. If there are multiple species of a given component, they are to be separated by a ‘.’ symbol (similar to reaction SMILES). Even though the representation of an electrolyte should be complete by encoding information of only solvents, salts, and additives, we also provide an option of entering information about experimental conditions at which the electrolyte measurements have been carried out (intensive variables) such as temperature, current density, and capacity. This information becomes crucial for electrolyte properties such as ionic conductivity, viscosity, Coulombic efficiency, etc. All such variables are to be separated by a ‘^’ sign.

**Note:** Choosing a standard unit for different components in the electrolyte SMILES can be critical – we can fix the above units to be standard, i.e., volume per volume for solvent ratio, molarity for salt concentration, and weight percent for additive amount. But users can be given the flexibility to enter electrolyte SMILES in units of their choice, e.g., volume/weight/molar ratios for solvent and additive amounts, and molarity/molality for salt concentration.