

**GLYCOL ETHERS AS PROMISING BATTERY ELECTROLYTES***Elbakari A.V., Emelyanov V.V., Vostrikov S.V., Verevkin S.P.*

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In recent decades, lithium-ion batteries have increasingly been used for efficient electrical energy storage. Solutions based on lithium salts and organic ether solvents are volatile, flammable, and unstable during long-term use. To address the challenges associated with lithium-metal batteries, several researchers have considered the use of electrolyte solutions based on glycol diesters, also known as "glymes" [1].

Glymes possess physicochemical properties that address the key challenges associated with lithium-metal batteries: liquid state over a wide temperature range, high chemical and thermal stability, relatively low vapor pressure, and low toxicity. This is particularly true for polyglycol diesters.

A challenge has been the lack of experimental thermodynamic data for long-chain glymes. Only the first four compounds in the homologous series have been thoroughly studied. Therefore, filling in these missing data is a priority for this study. Various approaches were used, including a combination of empirical methods (correlations using Kovacs indices, correlations with enthalpies of solution, etc.) and high-precision quantum chemical calculations (G3MP2, B3LYP with CREST conformational analysis) to predict enthalpies of vaporization, heat capacities, and Gibbs energies.

Experimental enthalpies of vaporization for a homologous series of ethylene glycol ethers were collected and validated using empirical methods: correlations using enthalpies of solution, the number of  $-\text{[O-CH}_2\text{-CH}_2\text{]}-$  units in the glyme molecule, Kovacs indices, surface tensions, boiling points, and Hildebrandt solubility parameters. The enthalpies and entropies of formation in the gas phase of ethylene glycol ethers were obtained using high-precision quantum chemical calculations. Using the enthalpies and entropies of formation in the gas phase and the enthalpy of vaporization, the enthalpies and entropies of formation in the liquid phase were calculated.

This yielded reliable thermodynamic data that were used to calculate the lower flammability limit, flash point, adiabatic temperature rise, and decomposition temperature. These parameters help evaluate the decomposition reaction and the thermal stability of glymes. The results suggest that glymes offer high safety and are promising electrolytes for batteries.

1. Brouillette D., Perron G., Desnoyers J. E. Apparent Molar Volume, Heat Capacity, and Conductance of Lithium Bis(trifluoromethylsulfone)imide in Glymes and Other Aprotic Solvents // *J. Solution Chem.* 1998. Vol. 27, P. 151–182.  
<https://doi.org/10.1023/A:1022609407560>

*Acknowledgments:* This work was supported by the Ministry of Science and Higher Education of the Russian Federation (theme № FSSE-2025-0006) as part of the state task of the Samara State Technical University.