Journal of Chemical&Engineering Data

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Submission Checklist

For additional details, see the **Author Guidelines**

Before submitting your manuscript to *JCED,* check your submission for the items below. The peer review process will be expedited if your manuscript adheres to the specific requirements for experimental and molecular modeling submissions.

Abstract

☐ Does the abstract clearly identify the chemical systems investigated, properties or phase equilibria studied, experimental and/or computational approaches used, and summarize the results? Is TOC graphic included?

Chemical Sample Table

☐ For identification, are IUPAC systematic names, CAS registry numbers, and 2D structures/CIF files provided for all chemical compounds and materials? At least two identifiers must be provided.

- For experiment, include source of chemicals, purification methods used, and final sample purity.
- For molecular modeling, include information on force field or electronic structure method.

Thematic Sections

☐ Does the manuscript adhere to the guidelines for the appropriate thematic section? Refer to **Thermophysical and Thermochemical Properties [PDF]**, **Vapor-Liquid Equilibria and Supercritical Fluid Equilibria [PDF]**, **Liquid-Liquid Equilibria and Vapor-Liquid-Liquid Equilibria [PDF]**, **Solid-Solid Equilibria and Solid-Fluid Equilibria [PDF]**, or **Adsorption and Diffusion in Porous Materials [PDF]**.

Data

☐ Does the main manuscript contain tables of all of the primary experimental or computational data? If representation of primary data through fitting to a thermodynamic model is an important part, then the model parameters should also be reported in the main manuscript.

☐ Are S.I units used throughout the text, tables, and graphics?

☐ In table and figure captions, are the system(s) and state point(s) clearly identified? (e.g., *T* and *P*) Are the compositions reported in appropriate units? (Note: Molarities and ppm are not allowed.)

Literature Comparison

☐ Has a search been performed for previously published experimental data (e.g., **Thermolit**) and computational data?

☐ Are comparisons made between new data reported in the manuscript and previously reported data including for sub-systems (e.g., binary sub-systems of a fluid ternary mixture or unary adsorption for multi-component mixture)? Are deviations from literature values shown as deviation plots? We encourage this comparison by plotting the difference between the new data and the literature values in either the manuscript or Supporting Information.

Molecular Modeling and Simulation [PDF]

☐ Are all computational algorithms and methods described in sufficient detail to allow calculations to be reproduced, and appropriate references provided? Data requiring proprietary algorithms and models should not be included.

Uncertainty

☐ Are statistical and method uncertainties provided? Are means for their calculation/estimation specified? Are data reported with either the standard uncertainty or the expanded uncertainty with the level of confidence specified (both absolute and relative uncertainties are acceptable)? (Note: For experimental data, uncertainties need to be provided for both measured values (e.g., viscosity) and for fixed variables (e.g., *T* and *P*)). More information on Reporting Uncertainty in Results can be found in **the Manuscript Components section of the Author Guidelines**.

☐ Have appropriate measurements of a reference system been performed and reported to verify reported uncertainties and to confirm the reliability of the apparatus or software? A reference system is one whose values have been measured and reported by numerous other researchers.

☐ Is the impact of sample purity on the uncertainties reported? (e.g., The instrument uncertainty of a vibrating tube densitometer may be 0.00005 g/cm^3, but the actual uncertainty is much greater if the sample is only 98% pure.)