**GUIDELINES FOR REPORTING OF NEW PROPERTY DATA OBTAINED FROM MOLECULAR MODELING AND SIMULATION**

The following is a list of the requirements for manuscripts reporting new property data obtained from molecular modeling and simulations (MMS) to be published in the *Journal of Chemical and Engineering Data*. It should be understood that this list is not exhaustive, but descriptive of the expectations for such manuscripts. Data reproducibility and veracity are of paramount interest for the *Journal of Chemical and Engineering Data*.

- **Article Title**
  - Presence of new MMS data in the article should be clear
  - Properties measured and the chemical systems should be named, if practical
  - Computational approaches should be named, if practical
- **Abstract**
  - Chemical systems and properties measured must be summarized
  - Computational approaches must be summarized
- **Chemical System Information**
  - IUPAC systematic name and chemical formula are required for all chemical compounds
  - Include structural drawings for complex molecules
  - Inclusion of the CASRN is optional, but highly recommended
  - Clear description of the system(s) and state point(s) (in accord with the Gibbs phase rule) investigated must be given; e.g., for a simulation in the canonical ensemble, specify the number of molecules for each compound, the volume for fluid phases or the simulation cell parameters for crystalline phases, and the absolute temperature
  - For manuscripts reporting data for multiple systems, a Table summarizing the chemical system information is encouraged
- **MMS: Software, Algorithms, Force Fields, Simulation Protocols, and Other Details**
  - Define all acronyms
  - Software
    - Commercial software and widely-distributed open-source software
      - Provide full detail that allows to identify the specific version of the software used
      - Provide references for key papers utilizing this software for related data prediction or report computations for well-characterized chemical or model (e.g., Lennard-Jonesium) systems to demonstrate performance
    - In-house software
      - Provide references for key papers utilizing this software for related data prediction or report computations for standard chemical systems to demonstrate performance
  - Computational Algorithms and Methods
    - Provide a short description with appropriate references to all computational algorithms and methods used (e.g., specify the integrator and, if applicable, thermostatting and barostatting approaches used for molecular dynamics simulations, or specify the theory behind electronic structure calculations)
  - Force Fields, Functionals, Basis Sets, and Pseudopotentials
    - Provide a short description with appropriate references to all force fields, functionals, basis sets, and pseudopotentials in the main manuscript
    - Provide complete detail of all of modeling parameters in the Supporting Information
      - For well-documented force fields, etc., the references may be sufficient but, if practical, then include tables listing these parameters or provide a suitable input file for a widely-distributed open-source software that contains all of these parameters
      - MMS data hinging on proprietary force fields, etc., are not reproducible or verifiable with other MMS approaches and are, hence, not suitable for publication in the *Journal of Chemical and Engineering Data*

        - Use of potential truncation and treatment of long-range interactions should be described in detail.
    - Simulation Protocols and Other Details
        - Provide a short description with appropriate references to simulation protocols and other details (e.g., generation of initial configuration (if applicable, including initial velocities), pseudo-random-number generator, time step or fraction of specific Monte Carlo moves, etc.) in the main manuscript
        - Provide complete detail of all of these simulation-protocol parameters in the Supporting Information
            - When using widely-distributed open-source software providing all input files is encouraged
        - For electronic structure calculations provide information on initial conformation/configuration and on whether multiple local minima on the potential energy surface are used for property calculation
    - Statistical and Method Uncertainties
        - Provide a detailed description of how statistical uncertainties were determined (e.g., using $N_{sample}$ independent simulations started from different initial configurations with equilibration and production periods consisting of $S_{equil}$ and $S_{prod}$ time steps or Monte Carlo moves); distinguish clearly between standard deviation (dependent on length of independent runs) and standard error of the mean (dependent on combined length of all independent runs)
            - If block averages are used, then provide details in the Supporting Information showing that blocks are uncorrelated, or that correlation is accounted for in the uncertainty estimates
        - Include discussion of the method uncertainty (e.g., force field parameters, system size, DFT functional, basis set)
- **Numerical MMS Results: <u>Stand-Alone Tables</u>**
    - If practical, data should always be reported in stand-alone tables in the main body of the manuscript; only when the amount of data is extraordinarily large, then it will be permissible to use figures in the main manuscript and include data tables in the Supporting Information
    - Examples of well-constructed stand-alone tables for common data types are available online: http://trc.nist.gov/JCED-Support.html
    - Terminology
        - Names of all properties, variables, and thermodynamic constraints (in accord with the Gibbs phase rule) should be written out in the table heading (e.g., temperature $T$, rather than simply $T$)
        - IUPAC (Green Book) recommendations must be followed
        - Only SI units should be used
    - Reporting of all Properties, Variables, Constraints
        - All values must be reported in accord with the Gibbs phase rule
        - Values of variables should not be implied, nor reported only in the text
    - Identification of Phases
        - All co-existing phases must be identified, including chemical identification of crystalline phases
    - Reporting of Composition
        - Mole fraction, mass fraction, or molality should be used
        - All compositions must be defined completely in the table
        - If molality is used, the solvent must be defined clearly
        - Amount concentration (formerly molarity) and volume fraction should not be used as expressions of composition. If used, mole fraction, mass fraction, or molality must also be given.
    - Uncertainties
        - Uncertainties *must be included in the data tables* for all properties and variables
            - Uncertainties can be included as footnotes or in the body of the table, as needed

        - For MMS data, uncertainties are usually not associated with the thermodynamic constraints
    - The standard uncertainty $u(\varphi)$ or relative standard uncertainty $u_r(\varphi) = u(\varphi)/|\varphi|$ must be included for all variables. (Here, $\varphi$ represents a variable.)
    - The combined (using propagation) expanded uncertainty $U(\varphi)$ or relative combined expanded uncertainty $U_r = U(\varphi)/|\varphi|$ (with level of confidence = 0.95 being strongly preferred) should be reported for properties
  - Derived Data
    - Reporting of primary MMS data and derived data in a single table should be limited to that required for the scientific discourse of the article
- Comparisons with Previously Published Data
  - Authors are expected to complete a detailed literature search
    - **Note 1:** The free online tool ***ThermoLit: The NIST Literature Report Builder for Thermophysical and Thermochemical Property Measurements*** is available to aid this process.
      **See:** http://trc.nist.gov/thermolit/
    - **Note 2:** This web application provides free and open access to literature information contained in the *NIST/TRC SOURCE Data Archive*, and provides an easy-to-use tool for generation of a *NIST Literature Report in PDF format*. The tool is intended to aid researchers and reviewers in determining relevant literature sources for a given experimental measurement; however, *it is not intended to replace the comprehensive literature review required by all journals*, and no guarantee is made regarding completeness of the information provided.
  - Comparisons must be provided with previously published values, where available
    - Comparisons for properties with state variables should be shown graphically in the form of absolute or relative deviations from a particular model or fitted equation
    - Comparisons should include, where available, published experimental *and* MMS data