GUIDELINES FOR REPORTING OF SOLUBILITY DATA

The following describes requirements necessary for manuscripts reporting solubility data of solid solutes in solvents or solvent mixtures to be published in the Journal of Chemical and Engineering Data JCED. These guidelines are given as a supplement to the general *Author Guidelines* for JCED (see http://pubs.acs.org/paragonplus/submission/jceaax/jceaax_authguide.pdf).

- Article Title
  - Name of the solute must be given, and the identity of the solvent(s) should be given, if practical. Abbreviations should not be used.
  - Temperature range of solubility measurements should be mentioned, if practical.
- Abstract
  - All of the following must be mentioned.
    - Chemical systems
    - Experimental methods
    - Variable ranges (temperature and pressure)
    - Modeling approaches
- Substance Information
  - Description of chemical substances must conform to the *Author Guidelines* cited above.
  - Melting temperature and melting enthalpy (with uncertainties), based on new measurements or from the literature, should be reported if possible.
- Experimental Data
  - The experimental method must be fully described and validated.
    - The method must be validated by measurements for, at least, one system for which multiple consistent data are available in the literature. The validation measurement results must be presented in tabular form, and deviation from literature values must be given in numerical or graphical form.
  - For the studied systems, graphical comparison must be provided for all available literature data, as described in the *Author Guidelines*.
  - Solubility data involving various polymorphs, amorphous solids, hydrates, complexes, *etc*., require experimental proof of the identity of the solid in equilibrium with the saturated solution (*e.g*., via x-ray diffraction).
  - The amount of experimental solubility data presented should be substantial.
    - Specifically, the number of solutes times the number solvents should be at least 12. (For example, 3 solutes in 4 solvents, or 2 solutes in 6 solvents.) A binary solvent system with results for at least three different solvent compositions, in addition to the pure solvents, counts as three solvents.
    - The temperature interval for solubility measurements should be at least 40K.

    - Experimental data are to be presented in stand-alone tables with complete uncertainty specification, as described in the *Author Guidelines*. Examples of complete and well formatted tables can be found online. (Example tables. See section 4 on the website; *Solid Liquid Equilibrium (SLE) Data*)
    - Experimental data need to be presented in figures, where plots of ln Y vs. T^{-1} (where Y is solubility expressed as mole fraction or molality) are required. Plots of Y vs. T may also be presented, if useful. (Figure examples are given below the table examples on the Journal-support website. Example figures.)

- Thermodynamic modeling of solubility data
    - It is preferred that solubility data be modeled using an activity-coefficient model (g^E-model or equation of state).
    - Model parameters must be presented in tables.
    - Deviations of experimental from correlated data should be tabulated with the experimental data.
    - Empirical correlation of experimental data is required only when thermodynamic modeling with activity coefficients is not performed.
    - A maximum of two empirical equations should be used for correlation.
    - Parameters of correlations should be reported in tables.
- Thermodynamic properties of dissolution
    - Using the van't Hoff equation to obtain standard properties of dissolution (entropy, enthalpy, and Gibbs energy of solution) is only valid for ideal solutions or at infinitely-low solute concentrations. It should, therefore, only be applied when accounting for the non-ideality of real systems using the solute activity coefficients. The latter should be obtained from a thermodynamic model (see previous section).