ThermoML: A New IUPAC Standard for Thermodynamic Data Communication

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ThermoML is a new XML-based IUPAC standard for storage and exchange of experimental, predicted, and critically evaluated thermophysical and thermochemical property data. The basic principles, scope, and description of all structural elements of ThermoML will be discussed. ThermoML covers essentially all thermodynamic and transport property data (more than 120 properties) for pure compounds, multicomponent mixtures, and chemical reactions (including change-of-state and equilibrium reactions). Representations of all quantities related to the expression of uncertainty in ThermoML conform to the *Guide to the Expression of Uncertainty in Measurement* (GUM). It will be shown that equations can be defined by any user of ThermoML through use of the *ThermoML-EquationDefinition* schema. By linking the *ThermoML-EquationDefinition* schema to MathML, it is possible to take advantage of the full scope of elements developed for MathML in construction of the equation definition. All definitions of the ThermoML are fully compliant with those of the IUPAC Green Book. The role of ThermoML in establishing a large-scale global data delivery process from the "data producers" to the "data users" will be illustrated.