

Provisional Recommendations

IUPAC Seeks Your Comments

Provisional recommendations are drafts of IUPAC recommendations on terminology, nomenclature, and symbols made widely available to allow interested parties to comment before the recommendations are finally revised and published in *Pure and Applied Chemistry*.



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JCAMP-DX for Electron Magnetic Resonance

In this document, we define a data exchange format initially formulated from discussions at the 35th Royal Society of Chemistry-ESR conference in Aberdeen 2002. The definition of this format is based on the IUPAC Joint Committee on Atomic and Molecular Physical Data Exchange (JCAMP-DX) protocols, which were developed for the exchange of infrared spectra and extended to chemical structures, nuclear magnetic resonance data, mass spectra and ion mobility spectra. This standard was further extended to cover year 2000 compatible date strings and good laboratory practice and the next release will cover the information needed for storing n-D data sets. The proposed recommendations aim at adapting JCAMP-DX to the special requirements for EMR, electron magnetic resonance.

Comments by 31 January 2006

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www.iupac.org/reports/provisional/abstract05/lancashire_310106.html

XML-Based IUPAC Standard for Experimental, Predicted, and Critically Evaluated Thermodynamic Property Data Storage and Capture (ThermoML)

ThermoML is an XML-based emerging 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 are 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). The ThermoMLEquation schema for representation of fitted equations with ThermoML is also described and provided as Supporting Information together with specific formulations for several equations commonly used in the representation of thermodynamic and thermophysical properties. The role of ThermoML in global data communication processes is discussed. The text of a variety of data files (use cases) illustrating the ThermoML format for pure compounds, mixtures, and chemical reactions, as well as the complete ThermoML schema text, are provided as Supporting Information.

Comments by 31 January 2006

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