NOMENKLATURA A TERMINOLOGIE

DOPORUČENÍ IUPAC

In this document, we define a data exchange format initially formulated from discussions of an IUPAC limited-term task group 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 of the JCAMP-DX 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 aim of this paper is to adapt JCAMP-DX to the special requirements for EMR, electron magnetic resonance.

Otiskujeme synopsi návrhu z oboru chemické informatiky, který byl připraven komitétem IUPAC pro tištěné a elektronické publikace. Návrh je nyní určen k posouzení a kritice chemické veřejnosti. Zájemci o bližší informace či o text návrhu se mohou obrátit na adresu Národního střediska IUPAC v České republice:

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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.

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