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Angela M. Hunter <angela.hunter@orglett.acs.org> is Data analyst, Organic Letters in the Department of Chemistry at the University of Pennsylvania, Philadelphia, USA. ORCID.org/0000-0002-3474-525X

Update on ThermoML

by Kenneth Kroenlein

ThermoML is the XML-based IUPAC Standard for Thermodynamic Property Data, first developed as an IUPAC project in 2006, and extended in 2001. [1] At present, ThermoML is being used by a number of process design packages as a data input format, as well as more broadly on the Internet as a data dissemination format. The freely-accessible ThermoML archive maintained by the Thermodynamics Research Center (TRC) is the primary source of these data and has new address <https://www.nist.gov/mml/acmd/trc/thermoml-archive>. We fully expect this archive to continue to grow as new materials as published.

The most recent development impacting ThermoML is the expansion of TRC's data collection activities into metal-based systems. Several elements of metals-based systems reporting requirements, around concepts such as phase description and differing expectations for sample characterization, made substantial update of the ThermoML schema necessary.

Accordingly, TRC is developing an updated schema, version 5.0, and associated forward and backward conversion software in the context of IUPAC.

Previous recommendations related to ThermoML:

- Frenkel, M. *et al.* XML-based IUPAC standard for experimental, predicted, and critically evaluated thermodynamic property data storage and capture (ThermoML) (IUPAC Recommendations 2006). *Pure Appl. Chem.* **78**(3):541-612, 2006, <https://doi.org/10.1351/pac200678030541>
- Frenkel, M. *et al.* Extension of ThermoML: The IUPAC standard for thermodynamic data communications (IUPAC Recommendations 2011). *Pure Appl. Chem.* 2011, **83**(10):1937-1969, <https://doi.org/10.1351/PAC-REC-11-05-01>

[1] <http://www.iupac.org/namespaces/ThermoML>

Kenneth Kroenlein <kenneth.kroenlein@nist.gov> is Group Leader, Thermodynamics Research Center, National Institute of Standards and Technology, in Broomfield, Colorado, USA.