

International Union of Pure and Applied Chemistry

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PROJECT SUBMISSION FORM

*v. August 2016*

Any individual or group can submit a project, with or without current affiliation with an IUPAC body. Projects can be submitted at any time. For detailed information, see the additional ***Guidelines for Completion of the Project Submission Form***. Frequently Asked Questions on ***Project Submission and Approval Process*** are also available on the Union’s web site at <http://www.iupac.org/projects>.

This form should be completed with a word processor and returned to the IUPAC Secretariat, preferably as an e-mail attachment to <secretariat@iupac.org>. Please do not remove section headers and answer all questions; indicate NA when a question does not apply to the proposal.

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| *for administrative use only* | | *Submitted \_\_\_\_\_\_\_\_\_\_\_\_\_\_ ; # \_\_\_\_\_\_\_\_\_\_\_\_\_* |
| **Date** | Monday, 17 April 2017 | |
| **Project Title** | ThermoML-2017 Revision of an XML based IUPAC Standard for Thermodynamic Property Data | |
| Series Title *(if applicable)* | XML-based IUPAC Standard for Experimental and Critically Evaluated Thermodynamic Property Data Storage and Capture | |
| **Task Group Chair** | Wilthan, Boris  Thermodynamics Research Center, 847.01  Physical and Chemical Properties Division  National Institute of Standards and Technology  325 Broadway  Boulder, Colorado 80305-3328  USA  [boris.wilthan@nist.gov](mailto:boris.wilthan@boulder.nist.gov) | |
| **Task Group** **Members** | Paul Mason  Thermo-Calc Software Inc.  4160 Washington Road  McMurray PA, 15317 USA  [paul@thermocalc.com](mailto:paul@thermocalc.com)  Ursula Kattner  Thermodynamics and Kinetics Group  Materials Measurement Laboratory  100 Bureau Drive M/S 8554  Gaithersburg, MD 20899  [Ursula.kattner@nist.gov](mailto:Ursula.kattner@nist.gov)  Kazuya Saito  University of Tsukuba  Faculty of Pure and Applied, Sciences  Tsukuba Campus, University of Tsukuba,  1Chome-1-1 Tennōdai, Tsukuba-shi, Ibaraki-ken305-0006, Japan  [kazuya@chem.tsukuba.ac.jp](mailto:kazuya@chem.tsukuba.ac.jp)  Nathalie  Dupin  Calcul Thermodynamique  3 rue de l’avenir  63670 Orcet France  [Nathdupin@wanadoo.fr](mailto:Nathdupin@wanadoo.fr)  Debbie Mies  Granta Design Ltd.  Cambridge, Cambridgeshire, UK  debbie.mies@grantadesign.com  Georg Schmitz  Lehr­stuhl für Me­di­zin­tech­nik Ge­bäu­de ID, Etage 04, Raum 231 Uni­ver­si­täts­str. 150 Ruhr-Uni­ver­si­tät Bo­chum 44801 Bo­chum  [Georg.schmitz@rub.de](mailto:Georg.schmitz@rub.de)  Kroenlein, Kenneth  Group Leader, Thermodynamics Research Center  National Institute of Standards and Technology  325 S Broadway  Broomfield, CO 80304  [Kenneth.kroenlein@nist.gov](mailto:Kenneth.kroenlein@nist.gov)  Ladbury, John  Department of Biochemistry and Molecular Biology, Center for Biomolecular Structure and Function  LC Miall 7.07 School of Molecular and Cellular Biology 011334335669 [j.e.ladbury@leeds.ac.uk](mailto:j.e.ladbury@leeds.ac.uk)  Heiko Heerklotz  Lehrstuhl für Pharmazeutische Technologie und Biopharmazie  Hermann-Herder-Straße 9  [heiko.heerklotz@pharmazie.uni-freiburg.de](mailto:heiko.heerklotz@pharmazie.uni-freiburg.de)  D-79104 Freiburg i. Br.  Robert Goldberg  National Institute of Standards and Technology  Bioassay Methods Group  100 Bureau Drive  Gaithersburg, MD 20899  [Robert.goldberg@nist.gov](mailto:Robert.goldberg@nist.gov)  John Dymond  [dunmorecot@tiscali.co.uk](mailto:dunmorecot@tiscali.co.uk) | |
| **Name** of the person submitting this form ***if not*** *the proposed Task Group Chair* | Erik Pfeif ([erik.pfeif@nist.gov](mailto:erik.pfeif@nist.gov) )  325 S. Broadway Boulder, CO 80305 | |
| **Objectives and Rationale**  (This should summarize the principal objectives and rationale, and the intended outcomes.)  *(see Guidelines)* | It is intended to update the XML-based dictionary for storage and exchange of thermophysical and thermochemical data based on fundamental principles of phenomenological thermodynamics covering a wide variety of systems such as pure chemical compounds, multicomponent mixtures, and chemical reactions.  Upon completion of the project, the developed dictionary and corresponding XML schema could become an internationally accepted standard for thermodynamic data storage and exchange.  The coverage of the XML standard must be expanded to provide a standard for the multitude of engineering applications and research projects that utilize data as a key element of design. | |
| **Intended Stakeholders**  (Give details of the intended stakeholders and interest groups, and how they will benefit from your Project Objectives.) *(see Guidelines)* | Stakeholders: Thermophysical property publishers; engineers; big-materials data, and individual researchers.  ThermoML, already endorsed by the five major scientific publishing journals in publishing of thermophysical and thermochemical property data, from which stakeholders can freely download data in ThermoML4.0 format via ThermoML Archive: (<https://www.nist.gov/mml/acmd/trc/thermoml-archive> )  The system has already benefitted the organic scientific and engineering communities around the world, and can be expanded upon. The same tools, used to increase data quality, communication, and standards will continue in use by organic scientific communities, and be expanded for use by metallurgical data users and producers.  In metallurgical realm, the data schema will aid in high throughput computational materials engineering, model description development for the CALPHAD community, metallurgists, and societies (ASM, AWS, SME) alike. | |

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| **Dissemination Plan**  (Indicate how the results of this Project will be communicated to target stakeholders and, if relevant (e.g. for IUPAC Recommendations), how the Task Group will involve stakeholders in the refinement of Project outcomes.) *(see Guidelines)* | This project will be disseminated through the same namespace ([www.iupac.org/namespaces/ThermoML/](http://www.iupac.org/namespaces/ThermoML/)) as was done prior.  The Task group will involve stakeholders in the following way:   1. A project task group meeting 2. A publication of a manuscripts to be published in    1. The Pure Appl. Chem. for the organics data producers and users    2. The CALPHAD Journal for the metallurgical data producers and users  for public review and comments for 3 months 3. At least two in-person meetings and three teleconferences will be held to work though necessary comments and reviews for modification |
| **Intended Publications**  (please tick boxes)  (*see Guidelines*) | IUPAC Recommendation 🗹  IUPAC Technical Report   Other type of manuscript to be published in a journal other than *Pure and Applied Chemistry* 🗹  *Specify:* …………………  Book  *[include any preliminary communication, draft agreements and intended publisher, if known]*  Workshop or conference proceedings   Set of instructional materials   Database 🗹  Web page 🗹 *[Any website/webpage intended to be on the IUPAC.ORG platform is required to be on WordPress platform and meet IUPAC’s guidelines for branding, hosting, and compatibility]*  Other: ………………… |

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| **Description**  *(see Guidelines)* | This project is to be considered as a REVISION of the 2002-055-3-024 “XML-based IUPAC standard for experimental and critically evaluated thermodynamic property data storage and capture”, which was successfully completed in 2006. From that project, a new XML-based IUPAC standard (ThermoML) was established for thermodynamic data communications (*Pure and Applied Chemistry*, **2006**, 78, 541-612).  Initially, ThermoML provided support for communications of experimental, critically evaluated, and predicted data for thermodynamic properties of pure and multi-component mixtures of molecular compounds with comprehensive representation of uncertainties (JCED, **2003**, 48, 2-13; **2003**, 48, 1344-1359; and **2004**, 49, 160-174). Prior to release as a standard, enhancements for aqueous electrolyte solutions and ionic liquids were included. In 2011, a revision was completed (IUPAC project 2007-039-1-024) which broadened the scope of ThermoML to support storage and exchange of thermodynamic property data for, (1) speciation and complex equilibria in aqueous and non-aqueous solvents, and (2) thermodynamic properties of biomaterials. Furthermore, the extension addressed experimental data in the primary literature, as well as derived equilibrium constants for reactions and the associated Gibbs energy, enthalpy and heat capacity data, including equation representation.  Thermodynamic property data for metallurgical systems play an essential role in Integrated Computational Materials Engineering and Design, which should be performed at the earliest stage of R&D. Yet, at present, there is no comprehensive data management system specifically designed for metallurgical data. This project will support communications for the prior properties and standards while expanding the XML for a few new properties, processing history metadata, and the phase characterization and assignment for thermophysical properties. |
| **Time Frame**  Planned start Date  Duration of Project | * April 2017 * 2 years |

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| **Milestones**  (Indicate the location, duration and approximate date of Task Group meetings, workshops, conference presentations, etc. and also the target dates for circulation of drafts and submission of final report.)  *(see Guidelines)* | April 2017—Submit Project Form document to IUPAC, assemble group, distribute rough draft of ThermoML for comments from task group members.  July/August 2017—Kick off teleconference depending on IUPAC acceptance  September 2017— Host in-person meeting/teleconference at European Conference on Thermophysical Properties in Graz, Austria (Sept. 2-8)  November 2017—Complete rough proposal of document  January 2017—Complete final draft  March 2018—Submit documents to journals for public commentary period  May 2018—End of commenting period.  Coordination teleconference for Symposium on Thermophysical Properties.  June 2018—Host in-person meeting/teleconference at the Symposium on Thermophysical Properties in Boulder, CO (June 24-29)  December 2018—Submit documents for publication in Pure Appl. Chem. and CALPHAD  April 2018—Establish ThermoML 5.0 namespace, release ThermoML 4.0-5.0 converter |

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| **Budget** Total from all sources | $14,000 |
| Travel (Provide a break-down of travel and *per diem* expenses for each meeting of the Task Group) | Kickoff- 0$  ECTP-$7,000  (2017 per diem rate: lodge: $202/night food: 139$/day)  STP- $7,000  (2017 per diem rate: lodge: $132/night food: 59$/day) |
| Administrative (Specify) | - |
| Other  (Specify) | - |
| **Total** (in USD) | $14,000 |
| Requested from IUPAC | $14,000 |
| Requested from other Sources  (Indicate sources and amounts) | - |
| **Criteria for Retrospective Evaluation of Outcomes and their Impact** | 1. Widespread use of the developed extensions for ThermoML by scientists and engineers worldwide 2. involvement of new journals in the ThermoML-based data exchange process 3. development of new ThermoML software “readers” in industry 4. Adaptation of existing infrastructure to new standard |
| **Relevant IUPAC Bodies**  (Please tick box/boxes.) | Physical and Biophysical x Inorganic  Organic and Biomolecular  Polymer  Analytical x Environmental  Human Health  Nomenclature   CHEMRAWN   Chemistry and Industry   Chemistry Education   Other ………………… |

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| **Suggested Referees** (Referees external to IUPAC) | (at least 3 names, including e-mail and postal addresses)  Sergei Decterov  Polytechnique Montreal  Department of Chemical Engineering  Member of Centre for Research in Computational Thermochemistry and Researcher  Quebec, Canada  [sergei.decterov@polymtl.ca](mailto:sergei.decterov@polymtl.ca)  Zi Kui Liu  Professor of Materials Science and Engineering  Pennsylvania State University  326 Steidle Building  University Park, PA 16802-5006  [liu@matse.psu.edu](mailto:liu@matse.psu.edu)  Laura Bartolo  Professor and Director, Center for Materials Informatics  Kent State University  036 Science Research Building  Kent, OH 44242-0001  [lbartolo@kent.edu](mailto:lbartolo@kent.edu)  Timothy Austin  Joint Research Centre  European Commission  Rue du Champ de Mars 21  1050 Brussels  Belgium  [Timothy.AUSTIN@ec.europa.eu](mailto:Timothy.AUSTIN@ec.europa.eu) |

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Guidelines for Completion of Project Submission Form

# Introduction

IUPAC has long been recognized as the world authority on chemical nomenclature, terminology, standardized methods for measurement, atomic weights and many other critically evaluated data. Projects sponsored by IUPAC should address one of these aspects of chemistry or one or more of the goals listed in the IUPAC Strategic Plan. The Strategic Plan can be downloaded from the IUPAC web site <<http://www.iupac.org>> or a copy can be requested from the Secretariat. After completion, **the Project Submission Form should be returned to the IUPAC Secretariat**, *not to any other person or body in IUPAC.* The Secretariat will initiate the review process, and communicate with the relevant IUPAC Body(ies).

While there is no set schedule for the evaluation process, it is *usually* not expected to take more than four months. Decisions will be taken during the course of the year as projects are submitted and the necessary information has been gathered. Frequently Asked Questions on ***Project Submission and Approval Process*** are also available on the Union’s web site at <http://www.iupac.org/projects>

# Guidelines

## Project Title

Short descriptive title of project. If applicable, specify ***Series Title***

## Task Group Chair

Name and affiliation of person(s) who will be coordinator for the project.

## Task Group Members

Names and affiliation of the task group members who have committed themselves and agreed to work on the project.

## Objectives and Rationale

In a few sentences (<100 words total) describe the rationale for the project, the objective(s) and the intended outcome(s). This statement should identify the benefits to the applicable chemistry community and the strategic value to IUPAC.

## Intended Stakeholders

It is important that your proposal clearly identifies the interest groups and stakeholders that will benefit from the project outcomes. In so doing it should also establish the need for the proposed project outcomes and identify the benefits to the stakeholders. The reviewers will look for strong links between the Dissemination Plan (next section) and the stakeholders who will benefit from the outcomes.

## Dissemination Plan

A good dissemination plan is a vital part of the project. The plan identifies how the project outcomes will be disseminated to the intended science community/stakeholders.

For example, will the selected publication vehicles, proposed workshops or conference presentations, enable a significant impact on the target group(s)?

In the case of nomenclature recommendations (including terminology, symbols, and units), how will these be made known to practitioners or to the intended audience? What plans have been made to promote international consensus?

## Intended Publications

Is the final product of the project a recommendation or report to be published in *Pure and Applied Chemistry,* in another journal or a book, as a workshop or conference proceeding, a set of instructional materials, a web page?

If a book (or editing of a book or chapter) is planned, please be clear about the status of the proposal with the intended publisher. Note that any publication contract or agreement must be made available to the Executive Director during the project review process. If a publisher has been approached, and a draft agreement developed, this should be included in the review packet. Technical Reports and Recommendations resulting from IUPAC Projects should be published in *Pure and Applied Chemistry*. The procedure is described in Appendix III of IUPAC Handbook *“Procedures for publications of IUPAC technical reports and recommendations*”, available online as at <http://iupac.org/what-we-do/recommendations/procedure-for-publication/>.

The Bureau has established a procedure to allow publication in other journals in exceptional circumstances where it can be demonstrated by the Task Group and the Division or Standing Committee that publication in another journal is in the best interests of IUPAC. Approval for such an exception should be requested by the Division President or Standing Committee Chair from the Secretary General. This request should explain why publication in another journal would be preferable to publication in *Pure and Applied Chemistry*.

For books, once the contract has been signed by the Executive Director and Secretary General,and before the final editing of an IUPAC-sponsored book, the manuscript must be reviewed by the ICTNS to establish conformity with IUPAC standards of terminology and nomenclature.

## Description

The description should be relatively brief (approx. 250 words) and should enable the reader to understand the methods (compilation, review, critical evaluation, consultation) used in the project. The description must make clear why the project should be carried out under the auspices of IUPAC.

The description should include a clear statement of (a) any previous or concurrent work done on the proposed project, including conferences or workshops; (b) any previous, concurrent or planned interactions with bodies outside IUPAC that are relevant to the project.

If it is considered necessary to provide additional background information and supporting documentation to permit proper evaluation of the proposal, this should be given on a separate sheet. For help in deciding what information to include, please consult the "*Advice for Project Reviewers*" at <http://www.iupac.org/projects>.

## Time Frame

Indicate the planned start and completion dates of the project. The anticipated duration of many IUPAC projects is two to three years. Longer term projects should be broken into phases. Each phase should have clearly defined and measurable outcomes. Projects need not conform to the IUPAC biennial budget cycle. That is, a project can begin at any time in one biennium and end in another.

## Milestones

Interim milestones, such as presentation of interim or final outcomes to a Conference or Workshop, completion of first drafts of a report, and indicative dates of task group meetings should be given. The intended location and duration of Task Group meetings should also be stated as this will have a bearing on the assessment of your proposed budget.

Major milestones such as target dates for completion of the final draft by the Task Group, assessment of external reviews of the draft, and submission of the final document should also be indicated.

Upon acceptance of the project, the milestones will be reviewed and a specific timeline for progress reports will be agreed on with the responsible Division or Standing Committee.

## Budget

The budget should justify all planned expenditure (from all sources) over the lifetime of the project. Costs for dissemination of the results should be included. These costs might include holding a workshop (*See note at the end for definition of a workshop*) or special symposium at a Conference to publicize the results of the project.

Travel expenses include total costs for attending meetings of the task group, according to the rules governing IUPAC expenses (Apex airfare, IUPAC *per diem* according to location). Because funds are limited, every effort should be made to utilize electronic communications in lieu of meetings of the task group.In view of the modern means of electronic communication, overhead expenses are expected to be minimal. However, in some cases, costs for meeting facilities, software development, technical assistance might be accepted. To rationalize costs, Task Groups will often meet in conjunction with a Conference which most might be attending. Note that Project funds must not be used to pay Conference Registrations, nor to facilitate attendance at a Conference. (An exception could be the attendance at a Conference by one member to make a project-based presentation on behalf of the Task Group.)

When the Task Group is seeking or has already received funding by other organizations and is approaching IUPAC for additional funding, these other organizations should be identified.

Please note that IUPAC projects can not be original research projects and the cost of new research work can not be a part of the project costs. In specific and well-documented cases, support for a workshop might be acceptable.

## Criteria for Retrospective Evaluation

How should the success of the project be measured and when?   
This will be evaluated with respect to the measurable impact of the outcomes on the identified stakeholders/interest groups. Another criterion might be: have the Recommendations been adopted by journals as part of their instructions for authors? How long after completion should it be possible to evaluate the impact of the project, and by what method(s)?

## Relevant IUPAC Bodies

Suggested Division(s) and/or Standing Committee(s) that should review this proposal and the final document (outputs), and will monitor progress of this project.

## Suggested Referees

Please suggest the names (and provide address, affiliation and e-mail) of at least three external referees who can be asked by the IUPAC Secretariat to evaluate the project. These referees are in addition to those from the lead Division/Standing Committee or from supporting Divisions/Standing Committees. Referees should be experts in the field, and in general be chosen so as to avoid the appearance of conflict of interest.

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**Definitions of Conference and Workshop**

The following definitions are used as guides in evaluating proposals for projects.

***Conference*** - a scientific meeting in which most participants take only a passive part in the program. Active participation is limited to the relatively few participants who present lectures or posters, chair sessions or ask questions.

Note that project funding is not intended to provide financial assistance to conferences or editing of proceedings of conferences. Under special circumstances, however, financial support for dissemination of the results of a conference may be provided. As an example, the conference may have addressed matters of global importance that result in important resolutions or other results.

***Workshop*** - a scientific meeting in which all participants are expected to take an active part in the program. Examples include, but are not limited to:

- formulation of ideas and initial plans for projects on specific topics;

- development of recommendations or reports on specific topics;

- critical review of recommendations or reports on specific topics;

- professional development courses involving hands-on experience in new instrumental, computational or evaluation techniques.

A workshop as a part of a project can cover different aspects, such as: project initiation, recruiting of task group members, draft report and consideration of public comments, presentation and dissemination of results. It is however expected that electronic communication will be used as much as possible in various steps of development of a project. Further, IUPAC will not fund a Workshop for the purpose of planning a project.