

Supporting Scientific Reviewing of Publications on Experimental Thermophysical and Thermochemical Research

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Thermophysical/thermochemical properties of chemical compounds, mixtures, and materials are widely used in various research fields (e.g., testing novel theories, resolving ambiguities, creation of correlations or predictive models), in industry (e.g., product design, chemical and safety engineering), and in education. This information is frequently obtained experimentally. A detailed analysis of thousands of publications in the field has shown that a significant part of such data is ambiguous or inadequate due to poor research design, experimental errors, and/or inappropriate reporting. In cooperation with chemical engineers, researchers, and data experts, the Thermodynamics Research Center at NIST has been involved in a series of IUPAC projects dedicated to supporting researchers at various stages, starting from experiment planning and validation of experimental methods to data reporting. For example, the principles of Good Reporting Practice (GRP) have been recently stated and justified in the IUPAC project "Good Reporting Practice for Thermophysical and Thermochemical Property Measurements" (IUPAC project #2019-013-1-10, <https://iupac.org/project/2019-013-1-100>).

In order to increase the impact of the GRP principles and foster their implementation, creation and dissemination of checklists and other tools supporting a scientific review process is planned as another IUPAC project (# 2023-008-1-024, <https://iupac.org/project/2023-008-1-024>). The checklists will include common sections, covering identification of studied compounds, properties, and methods, as well as specific details for different types of measurements (sections covering models may be included as an extension of the project). Development of an easy-to-navigate web interface to find relevant lists and collect observations is expected as a project output. The checklists are expected to make the work of reviewers easier, reveal and fix typical deficiencies prior to publication, improve the quality of scientific publications in the field, and assure complete and unambiguous data reporting. They can be mirrored by interested parties (universities, publishers, professional societies, and funding agencies). The project is still open for contributions from interested experts.