

Guidelines for Reporting of Phase Equilibrium Measurements (IUPAC Recommendations 2012)

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The critical importance of phase equilibrium properties in the development and optimization of numerous industrial processes is well established, particularly with regard to separation methods, such as distillation, extraction, and crystallization. This article includes recommendations for the reporting in the primary scientific literature of measurements involving phase equilibrium. The focus is on documentation issues, and many of the recommendations may also be applied to the more general fields of thermodynamic and transport properties.

This work builds upon earlier related efforts that span approximately 60 years. Especially in the last 20 years, several important and inter-related developments make imperative revision of the guidelines published previously [*Pure Appl. Chem.* 29, 395 (1972) and CODATA Bull. 21, 69 (1989)]. These developments include advances in the establishment of international standards for (1) evaluation and reporting of uncertainties (Guide for the Estimation of Uncertainty in Measurement, known as “GUM”); (2) terminology in physical chemistry (*Quantities, Units, and Symbols in Physical Chemistry*, also known as the “Green Book”); and (3) storage and exchange of experimental, predicted, and critically evaluated thermophysical and thermochemical property data (ThermoML). The present work is also motivated by major advances in electronic databases for thermophysical properties. In particular, procedures have been developed involving cooperation between the U.S. National Institute of Standards and Technology and journal editors and publishers to allow data reported in key journals to be easily incorporated into electronic databases and process simulation software without significant manual intervention. A further need for the present work stems from the rate of publication of phase equilibrium and property data that annually continues to increase, more than doubling in the last 10 years.

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Characterization of Photoluminescence Measuring Systems (IUPAC Technical Report)

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Despite the widespread and increasing use of photoluminescence measuring techniques in materials science, (bio)analytical chemistry, medical diagnostics, and biotechnology, many method-inherent problems are often neglected, resulting in measurements that are unreliable and of poor quality. These problems include, e.g., the nonlinearity of the detection system, and spectral bandpass-, detector voltage- and polarization-dependent effects. Furthermore, the general need for correction of measured signals for unwanted contributions from instrument-dependent effects that are wavelength-, polarization-, and time-dependent is frequently underestimated despite the significant distortions in spectral shape and intensity that are often introduced. These luminescence-inherent drawbacks hamper the reliability of photoluminescence data, the comparability of measurements between instruments, and quantification from measured fluorescence intensities as well as the determination of relative fluorescence quantum yields.

These demands enhance the need for internationally accepted procedures for instrument calibration and instrument performance validation (IPV) in conjunction with suitable standards.

To improve the overall reliability and comparability of fluorescence measurements, the purpose of this document is to present and discuss procedures for the characterization and performance validation of photoluminescence measuring systems. Special emphasis is dedicated to steady-state measurements of photoluminescence in solution and monochromator-based systems such as are most commonly found in research-grade instrumentation. The aim of this report is also to increase the awareness for the importance of a reliable instrument characterization and to improve the reliability and comparability of measurements of photoluminescence.

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