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Standards in biothermodynamics☆, ☆☆

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Abstract
The field of biothermodynamics encompasses physical property measurements on biochemical and biological systems. This chapter reviews the status of standards documents that are pertinent to biothermodynamics as well as recommendations that have been made for the reporting of experimental results. The importance of standards in nomenclature, symbols, units, and uncertainties is discussed and a summary of sources of data for biochemical substances and reactions is given.

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Introduction

Thermodynamic measurements on biochemical and biological systems are of fundamental scientific importance. Since the aim of these measurements is to obtain reliable values of physical properties, it is important for workers in this area to be aware of documents that provide guidance for the performance of these measurements and for the reporting of results. When documents of this sort carry the imprimatur of a well-known scientific or standards organization, these documents serve as *de facto* standards for this community of researchers. It is the aim of this chapter to summarize briefly the status of the standards documents that are pertinent to biothermodynamics as well as recommendations that have been made for the reporting of experimental results. In its broadest sense, the field of biothermodynamics encompasses all physical property measurements on biochemical and biological systems. However, since equilibrium and calorimetric measurements have been of primary interest in this field, properties that fall into these two categories have received the most attention in the literature and in the standards documents.

Nomenclature, symbols, units, and uncertainties

The effective communication of scientific information is enhanced by the use of a standard set of nomenclature, symbols, and units. For example, it would be difficult and confusing to read a publication in which the symbol *S* was used for equilibrium constant and the symbol *K* was used for entropy or if the symbol *Z* was used for pH. The problem would be compounded if the aforementioned properties were referred to by names that are not commonly used. Additionally, while several historical units such as British Thermal Units, pounds, and miles have their place, they have generally been replaced in the scientific literature and in most countries by the International System of units (SI) (Bureau International des Poids et Mesures, 2006).[1] Just as writers should rely on a dictionary, thesaurus, and style guide, researchers should rely upon a "language of science" (Mills, 1997) for effective communication. The need for standards in scientific communication has grown even more pressing as values of physical properties, i.e. data, are now being incorporated in large-scale efforts such as the Brenda (Schomburg et al., 2000) and Sabio-RK (Wittig et al., 2012) databases. Additionally, the entries in these databases are often used for calculations of other properties and for further applications which impact progress in science, health, and the economy. Thus, standards are needed in essentially all areas of science.

The most useful and definitive source of information on nomenclature for quantities, symbols, and units pertinent to physical chemistry is *Quantities, Units and Symbols in Physical Chemistry* (Cohen et al., 2007). This publication, which was prepared under the auspices of the Union of Pure and Applied Chemistry (IUPAC), traces its origin to the *Manual of Symbols and Terminology for Physicochemical Quantities and Units*, which was prepared in 1970. There have been several editions published between the 1970 Manual (McGlashan, 1970) and the most recent edition of *Quantities, Units and Symbols in Physical Chemistry* (Cohen et al., 2007). Since all of these editions have been published with a green cover, the publication is often referred to as the *Green Book*. The current edition of the *Green Book* (Cohen et al., 2007) is broad in scope and covers a wide variety of topics such as mechanics (classical and quantum), electricity and magnetism, spectroscopy, electromagnetic radiation, general chemistry, thermodynamics, kinetics, and transport properties.

Of fundamental importance to science and to the system of units are the concept of measurement and the use of quantity calculus. The system of SI units is based on seven base quantities: length, mass, time, electric current, thermodynamic temperature, amount of substance, and luminous intensity. All other physical quantities are derived from these base quantities. Physical quantities are represented as the product of a number and a unit and they follow the rules of mathematics. Thus, if the concentration of a solute is $c = 0.0010\ \text{mol dm}^{-3}$, one can write $c/(\text{mol dm}^{-3}) = 0.0010$ or $10^3 c/(\text{mol dm}^{-3}) = 1.0$. In the last two representations, the right side of the equation is a number. This emphasizes the fact that the result of an experiment is a ratio of the measured quantity to the value of some standard quantity, which, in this case is $1.0\ \text{mol dm}^{-3}$. In some usage, one sees $c\ (\text{mol dm}^{-3}) = 0.001$. However, it is formally incorrect. While there is little chance of confusion in this case, confusion arises often in regards to powers of 10 in table headings. For example, using the previously used value of *c*, if one were to write $10^{-3} c = 1.0$, one formally has $c = 1000\ \text{mol dm}^{-3}$. The author has seen this type of confusion many times in the literature and it is not always easy to determine the intent of the author(s) of the publication.

Clearly, the result of a measurement is significantly enhanced by a statement of its reliability or uncertainty. The uncertainty can be evaluated by the use of statistical methods and by a consideration of the possible systematic errors that might be associated with the measurement(s). Guidance on the estimation of uncertainties can be found in the *Guide to the expression of uncertainty in measurement* (1995) and in *Guidelines for evaluating and expressing the uncertainty of NIST measurement results* (Taylor and Kuyatt, 1994). When assigning uncertainties to measurement results in a publication, it is critical to also give the basis for these uncertainties.

Standards documents in biothermodynamics

Several standards documents that are specifically intended for the field of biothermodynamics have been published. Included in these documents are discussions of the fine points of experiments such as useful test reactions as well as guidance and recommendations regarding nomenclature,

[1] The thermochemical calorie, which is defined by the relation 1 cal = 4.184 J (Cohen et al., 2007), is a unit that still persists in the literature. The reasons for this are its long history and the fact that some scientific software uses the calorie rather than the joule. However, most calorimeters are calibrated by means of electrical energy, which implicitly has units of joules. Then, if one chooses to use calories, one must change the result of the calibration, already done in terms of joules, to calories. Thus one must perform an extra computational step in order to use a unit that has been obsolete for many years.