The International Association for the Properties of Water and Steam

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Guideline on the Use of Fundamental Physical Constants
and Basic Constants of Water

This guideline contains 7 pages, including this cover page.

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Further information about this guideline and other documents issued by IAPWS can be obtained from the Executive Secretary of IAPWS, or on the IAPWS Website at http://www.iapws.org.

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1 Introduction

The purpose of this Guideline is to set forth a consistent set of recommendations for best practice in the use of various fundamental quantities in IAPWS Releases and Guidelines. Additionally, this Guideline is available for others who may wish to make their scientific or engineering work as consistent as possible with IAPWS and other standards.

Section 2 contains recommendations for use of fundamental physical constants. Section 3 contains recommendations for molecular-level properties of water. Section 4 contains recommendations for thermophysical properties at unique physical states and states that are widely used as calibration standards. The recommendations in this Guideline are primarily for ordinary water, but some recommendations for heavy water are included.

The background information for most of these recommendations is given in Reference [1].

2 Physical Fundamentals

2.1 Fundamental Physical Constants

The international body CODATA determines accepted values of fundamental physical constants (such as the molar gas constant, Boltzmann's constant, and the unit electronic charge) at periodic intervals. IAPWS recommends that scientific work use the most recent CODATA values of these constants available at the time the work is performed. As of this writing, the most recent CODATA adjustment of values for physical constants is their 2006 adjustment [2]. The CODATA values are also available on the World Wide Web at: http://physics.nist.gov/cuu/Constants/index.html.

2.2 Temperature Scale

IAPWS recommends that scientific work use the most recent representation of the temperature scale as adopted by the International Committee for Weights and Measures (CIPM). As of this writing, the current standard is the International Temperature Scale of 1990 (ITS-90) [3].

Where possible, especially for precise measurements, data should be converted to the current temperature scale before being used to produce correlations, etc. Equations for converting temperatures to ITS-90 from its predecessor, the International Practical Temperature Scale of 1968 (IPTS-68) are given by Rusby [4, 5]. Conversion to IPTS-68 from its predecessor, IPTS-48, is described by Bedford and Kirby [6].

3 Molecular Properties

3.1 Isotopic Composition

We define the isotopic composition of "ordinary water substance" to be that of Vienna Standard Mean Ocean Water (VSMOW), which is documented in [7]. The isotopic composition of VSMOW is as follows [8]: the amount of ^{2}H is 0.015 574(5) atom percent of the total hydrogen, and the amounts of the total oxygen as ^{17}O and ^{18}O are 0.037 90(9) and 0.200 04(5) atom percent, respectively. The numbers in parentheses reflect the uncertainties in the last digit.

There may be situations (for example, in analysis of specific experiments) in which the isotopic composition is known to be different from that of VSMOW. In such cases, it would be appropriate to use that known composition in calculations such as conversion of data between mass-based and molar units.

3.2 Relative Molar Mass of Ordinary Water Substance

The relative molar mass used in calculations (with the exception, mentioned above, of cases in which the isotopic composition is known to be different) should be that of VSMOW. This is computed by combining the isotopic composition of VSMOW with the accepted values of the masses of each isotope. Performing this calculation with the 2003 atomic mass evaluation [9] yields a relative molar mass of 18.015 268, with an uncertainty of no greater than two in the last digit.

3.3 Relative Molar Mass of Heavy Water

We define "heavy water" as water whose hydrogen content is pure ^2H and whose oxygen has the isotopic composition of VSMOW [10]. The computation then proceeds in the same manner as for ordinary water, yielding a relative molar mass of 20.027 508, with an uncertainty of no greater than two in the last digit.

3.4 Dipole Moment

For purposes of making a standard definition, we consider the dipole moment of an isolated, nonrotating water molecule in its ground vibrational state. This is different from the "equilibrium" dipole moment sometimes discussed in the literature; the equilibrium moment is a hypothetical value which would be obtained in the absence of any vibration, ground state or otherwise.

We accept the results of Shostak et al. [11] who measured a dipole moment of 1.854 98(9) debyes for H_2O. They also measured the dipole moment for the HDO molecule (where D is deuterium, ^2H) in the ground state; this was 1.8517(5) debyes.

In order to get an effective dipole moment value for "ordinary water substance," one should average the moments of H_2O and HDO according to the isotopic composition of the hydrogen in VSMOW. In this case, the amount of ^2H is sufficiently small that the average is indistinguishable from that for H_2O. Therefore, for the dipole moment of the isolated water molecule in its ground vibrational state, we adopt the value 1.854 98(9) debyes. In SI units, this is $6.1875(3) \times 10^{-30}$ C·m.

3.5 Polarizability

The dipole polarizability of water is not a single number but rather a tensor. Because the anisotropy of water's polarizability is relatively small, it is a fair approximation for many purposes to ignore the anisotropy and use only the mean polarizability, which is one-third of the trace of this tensor. We consider only the mean polarizability here. It is common practice to tabulate not the polarizability α itself, but rather the combination $\alpha/4\pi\varepsilon_0$ (where ε_0 is the permittivity of free space), which has dimensions of volume. We adopt that convention here; if α itself is required, the value of ε_0 adopted by CODATA (see section 2) should be used in the conversion.

The polarizability is also frequency-dependent; we consider here the high-frequency (electronic) value and the low-frequency (static) limit. The latter includes not only the response of the electrons to an applied field but also a vibrational contribution from the response of the atoms in the molecule. For the mean electronic polarizability, we adopt the value $1.457(3) \times 10^{-30}$ m^3, which Russell and Spackman [12] extracted from refractive index data. For the vibrational contribution to the total polarizability in the low-frequency limit, we adopt the estimate of Bishop and Cheung [13], which is 0.037×10^{-30} m^3. The uncertainty in the vibrational contribution is probably on the order of ten percent [13]. For the mean total dipole polarizability (in the static limit), which is the sum of the electronic and vibrational effects, we therefore adopt a value of $1.494(7) \times 10^{-30}$ m^3.

4 Reference Thermophysical Quantities

4.1 Critical Constants

IAPWS standards exist for water's critical temperature, pressure, and density [14]. These values (T_c = 647.096 K, p_c = 22.064 MPa, ρ_c = 322 kg/m^3) should be uniformly used. For heavy water, values (T_c = 643.847 K, p_c = 21.671 MPa, ρ_c = 356 kg/m^3) are given in the same document. Where it is necessary to consider uncertainties in the values, those listed in the IAPWS release should be used.

4.2 Triple Point

The triple-point temperature of ordinary water is used to define the base SI unit of temperature, the kelvin, and is 273.16 K. For the triple-point pressure, we recommend the value measured by Guildner et al. [15], which is (611.657 ± 0.010) Pa.

4.3 Density Maximum

Liquid water at atmospheric pressure (0.101 325 MPa) has a maximum density at a temperature slightly below 4 °C. This point is often recommended as a reference standard for precise density measurement. The CCM (Consultative Committee for Mass and Related Quantities) of the CIPM (Comité International des Poids et Mesures) has adopted a value for this maximum density (for the isotopic composition of VSMOW) as a part of its standard table for temperatures from 0 °C to 40 °C [16]. This value is (999.974 95 ± 0.000 84) kg/m^3.

4.4 Reference Liquid Viscosity

The dynamic viscosity of liquid water at 101.325 kPa and 293.15 K is an important calibration standard. The International Organization for Standardization (ISO) [17] has accepted the value of 1.0016 mPa·s for this reference value, with an estimated uncertainty of 0.17 %.

5 References

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