

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

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Summary

This Guideline exists in order to provide a consistent set of recommendations for the use of fundamental physical quantities in IAPWS documents. It may also be useful for others who wish to make their work as consistent as possible with IAPWS and other standards.

This Guideline contains 7 pages, including this cover page.

Further information about this Guideline and other documents issued by IAPWS can be obtained from the Executive Secretary of IAPWS (Dr. D.G. Friend, dg.friend@iapws.org), or from <https://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 many of these recommendations is given in Reference [1].

2 Physical Fundamentals

2.1 Fundamental Physical Constants

The international body CODATA reports accepted values of fundamental physical constants at periodic intervals. This includes constants that are now fixed as part of the SI unit system (such as the molar gas constant and the Boltzmann constant) and those that are determined based on evaluation of data (such as the vacuum electric permittivity). 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 report of values for physical constants is their 2022 adjustment [2].

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]. Conversions from earlier scales, along with other considerations for the effects of temperature scales on thermophysical properties, are described by Harvey [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].¹ The isotopic

¹ Due to exhaustion of the original VSMOW sample, the International Atomic Energy Agency has prepared a new standard called VSMOW2 for calibration of measurements of isotopic composition. The isotopic composition of VSMOW2 is identical to that of VSMOW within measurement uncertainty. For more details, see <https://analytical-reference-materials.iaea.org/vsmow2>.

composition of VSMOW is as follows [8]: the amount of ^2H 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 2020 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

We first consider the dipole moment of an isolated water molecule in its ground rotational and vibrational state. We accept the results of Shostak *et al.* [11] who measured a dipole moment of 1.854 98(9) debyes for H_2O in its ground state. 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. The average dipole moment at finite temperature will be slightly different due to the occupation of higher rovibrational states; this temperature dependence has been described by Garberoglio *et al.* [12].

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 state, we adopt the value 1.854 98(9) debyes. In SI units, this is $6.1875(3) \times 10^{-30} \text{ C}\cdot\text{m}$.

3.5 Polarizability

The dipole polarizability of a water molecule 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 $\alpha/4\pi\epsilon_0$

(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 [2] should be used in the conversion.

The polarizability is also frequency-dependent; we consider here the electronic value that provides the only contribution at high frequency, and also the low-frequency (static) limit that includes not only the response of the electrons to an applied field but also a purely vibrational contribution from the response of the atoms in the molecule. For the mean electronic polarizability, extrapolation to zero frequency of precise refractivity data near 293 K [13, 14] produces $1.455 \times 10^{-24} \text{ cm}^3$. The standard uncertainty seems to be on the order of 0.3 %. The pure vibrational contribution to the polarizability in the low-frequency limit is approximately $0.041 \times 10^{-24} \text{ cm}^3$ [12]. With this addition of the vibrational contribution, the mean total static dipole polarizability near 293 K can be stated as $1.496(5) \times 10^{-24} \text{ cm}^3$. As with the dipole moment, the average polarizability depends weakly on temperature; a correlation for this dependence (in terms of the contribution to the first dielectric virial coefficient; this contribution is directly proportional to the polarizability) is given in [12].

4 Reference Thermophysical Quantities

4.1 Critical Constants

IAPWS standards exist for water’s critical temperature, pressure, and density [15]. These values ($T_c = 647.096 \text{ K}$, $p_c = 22.064 \text{ MPa}$, $\rho_c = 322 \text{ kg/m}^3$) should be uniformly used. For heavy water, values ($T_c = 643.847 \text{ K}$, $p_c = 21.671 \text{ MPa}$, $\rho_c = 356 \text{ kg/m}^3$) 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 was previously used to define the base SI unit of temperature, the kelvin, and was assigned a value of 273.16 K. In the “new SI” adopted in 2019 [16], the Boltzmann constant is fixed and the triple-point temperature is no longer exact, but the current best estimate, and the value assigned on the ITS-90, is still 273.16 K. For the triple-point pressure, we recommend the value measured by Guildner *et al.* [17], which is $(611.657 \pm 0.010) \text{ Pa}$.

4.3 Density Maximum

Liquid water at the standard atmospheric pressure p_0 , where $p_0 = 0.101\,325 \text{ MPa}$, has a maximum density at a temperature near 3.98 °C [18]. This density 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 [18]. This value is $(999.974\,95 \pm 0.000\,84) \text{ kg/m}^3$.

4.4 Reference Liquid Viscosity

The viscosity of liquid water at p_0 and 293.15 K is an important calibration standard. The International Organization for Standardization (ISO) [19] has accepted the value of 1.0016 mPa·s for this reference value, with an estimated uncertainty of 0.17 %.

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