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Revised Release on the Equation of State 2006 for H_2O Ice Ih

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This release replaces the corresponding release of 2006 and contains 12 pages, including this cover page.

This release has been authorized by the International Association for the Properties of Water and Steam (IAPWS) at its meeting in Arnhem, The Netherlands, 6-11 September, 2009, for issue by its Secretariat. The members of IAPWS are: Britain and Ireland, Canada, the Czech Republic, Denmark, France, Germany, Greece, Japan, Russia, the United States of America, and associate members Argentina and Brazil, Italy, and Switzerland.

In this release, including the title, H_2O is used to represent the description *ordinary water substance*. The equation of state for H_2O ice Ih provided in this release is a fundamental equation for the Gibbs energy as a function of temperature and pressure; details of the equation can be found in the article "A New Equation of State for H_2O Ice Ih" by R. Feistel and W. Wagner [1]. This equation of state provides the most accurate representation of the thermodynamic properties of the solid-phase ice Ih of H_2O over the entire existence range of ice Ih. As a result of a minor adjustment of the coefficient g_{00} given in Table 2, the revised equation improves numerical consistency [2] with the IAPWS-95 formulation for the fluid phase of water. Further information about this release and other releases issued by IAPWS can be obtained from the Executive Secretary of IAPWS or from http://www.iapws.org.

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1 Nomenclature

Symbol	**Physical quantity**	**Unit**
c_p	Specific isobaric heat capacity of ice	J kg^{-1} K^{-1}
$\mathrm{d}p_{\mathrm{melt}}/\mathrm{d}T$	Clausius-Clapeyron slope of the melting curve	Pa K^{-1}
f	Specific Helmholtz energy of ice	J kg^{-1}
g	Specific Gibbs energy of ice	J kg^{-1}
g^{L}	Specific Gibbs energy of liquid water on melting line	J kg^{-1}
g^{V}	Specific Gibbs energy of water vapor on sublimation line	J kg^{-1}
g_0	Residual Gibbs energy, Table 4	J kg^{-1}
$g_{00}\ldots g_{04}$	Real constants, Table 2	J kg^{-1}
h	Specific enthalpy of ice	J kg^{-1}
Δh_{melt}	Specific melting enthalpy	J kg^{-1}
Δh_{subl}	Specific sublimation enthalpy	J kg^{-1}
k	Uncertainty coverage factor	
p	Pressure	Pa
p_0	Normal pressure, p_0 = 101 325 Pa	Pa
p_{melt}	Melting pressure	Pa
p_{subl}	Sublimation pressure	Pa
p_{t}	Experimental triple-point pressure, p_{t} = 611.657 Pa	Pa
$p_{\mathrm{t}}^{\mathrm{num}}$	Numerical triple-point pressure, $p_{\mathrm{t}}^{\mathrm{num}} = 611.654\,771\,007\,894$ Pa	Pa
r_1	Complex constant, Table 2	J kg^{-1} K^{-1}
r_2	Complex function, Table 4	J kg^{-1} K^{-1}

Symbol	Physical quantity	Unit
r_{20} … r_{22}	Complex constants, Table 2	J kg^{-1} K^{-1}
s	Specific entropy of ice	J kg^{-1} K^{-1}
s^{L}	Specific entropy of liquid water	J kg^{-1} K^{-1}
s_0	Residual entropy, Table 2	J kg^{-1} K^{-1}
T	Absolute temperature (ITS-90)	K
T_{melt}	Melting temperature of ice	K
T_{melt,p_0}	Normal-pressure melting temperature, T_{melt,p_0} = 273.152 519 K	K
T_{t}	Triple-point temperature, T_{t} = 273.16 K	K
t_1, t_2	Complex constants, Table 2	
u	Specific internal energy of ice	J kg^{-1}
u^{L}	Specific internal energy of liquid water	J kg^{-1}
U	Expanded uncertainty	
u_{c}	Combined standard uncertainty	
v	Specific volume of ice	m^3 kg^{-1}
z	Any complex number	
α	Cubic expansion coefficient of ice	K^{-1}
β	Pressure coefficient of ice	Pa K^{-1}
κ_s	Isentropic compressibility of ice	Pa^{-1}
κ_T	Isothermal compressibility of ice	Pa^{-1}
π	Pi, π = 3.141 592 65…	
π	Reduced pressure, $\pi = p / p_{\mathrm{t}}$	
π_0	Reduced normal pressure, $\pi_0 = p_0 / p_{\mathrm{t}}$	
ρ	Density of ice	kg m^{-3}
τ	Reduced temperature, $\tau = T / T_{\mathrm{t}}$	

2 Introductory Remark and Special Constants

The numerical values of special constants used in the equation of state for ice Ih of H_2O are listed in Table 1. The term “Ih” means ice of the modification Ih with hexagonal crystals

TABLE 1 Special constants and values used in this release

Quantity	Symbol	Value	Unit	Reference
Experimental triple-point pressure	p_{t}	611.657	Pa	[3]
Numerical triple-point pressure	$p_{\mathrm{t}}^{\mathrm{num}}$	611.654 771 007 894	Pa	[2]
Normal pressure	p_0	101 325	Pa	[4]
Triple-point temperature	T_{t}	273.16	K	[5]

corresponding to the naturally abundant form of ice. For simplification, in the following the supplement “Ih” will be omitted at most places; when the term “ice” is used, “ice Ih” is always meant.

3 The Equation of State

The equation of state presented here is in the form of the Gibbs energy as a function of temperature and pressure, $g(T,p)$, corresponding to a Gibbs potential function. This equation of state for ice is given by Eq. (1) as a function of temperature, with two of its coefficients being polynomial functions of pressure,

$$
\begin{aligned}
g(T,p) &= g_0(p) - s_0 T_t \tau + T_t \,\mathrm{Re}\left(\sum_{k=1}^{2} r_k \left[(t_k - \tau)\ln(t_k - \tau) + (t_k + \tau)\ln(t_k + \tau) - 2t_k \ln t_k - \frac{\tau^2}{t_k} \right] \right) \\
g_0(p) &= \sum_{k=0}^{4} g_{0k} (\pi - \pi_0)^k \qquad (1) \\
r_2(p) &= \sum_{k=0}^{2} r_{2k} (\pi - \pi_0)^k ,
\end{aligned}
$$

with the reduced temperature $\tau = T/T_t$, the reduced pressure $\pi = p/p_t$, and the reduced normal pressure $\pi_0 = p_0/p_t$, where T_t, p_t, and p_0 are given in Table 1. The real constants g_{00} to g_{04} and s_0 as well as the complex constants t_1, r_1, t_2, and r_{20} to r_{22} are listed in Table 2.

TABLE 2 Coefficients of the equation of state (Gibbs potential function) as given by Eq. (1)

Coefficient	Real part	Imaginary part	Unit
g_{00}	$-0.632\,020\,233\,335\,886 \times 10^{6}$		J kg^{-1}
g_{01}	$0.655\,022\,213\,658\,955$		J kg^{-1}
g_{02}	$-0.189\,369\,929\,326\,131 \times 10^{-7}$		J kg^{-1}
g_{03}	$0.339\,746\,123\,271\,053 \times 10^{-14}$		J kg^{-1}
g_{04}	$-0.556\,464\,869\,058\,991 \times 10^{-21}$		J kg^{-1}
s_0 (absolute)	$0.189\,13 \times 10^{3}$		J kg^{-1} K^{-1}
s_0 (IAPWS-95)	$-0.332\,733\,756\,492\,168 \times 10^{4}$		J kg^{-1} K^{-1}
t_1	$0.368\,017\,112\,855\,051 \times 10^{-1}$	$0.510\,878\,114\,959\,572 \times 10^{-1}$	
r_1	$0.447\,050\,716\,285\,388 \times 10^{2}$	$0.656\,876\,847\,463\,481 \times 10^{2}$	J kg^{-1} K^{-1}
t_2	$0.337\,315\,741\,065\,416$	$0.335\,449\,415\,919\,309$	
r_{20}	$-0.725\,974\,574\,329\,220 \times 10^{2}$	$-0.781\,008\,427\,112\,870 \times 10^{2}$	J kg^{-1} K^{-1}
r_{21}	$-0.557\,107\,698\,030\,123 \times 10^{-4}$	$0.464\,578\,634\,580\,806 \times 10^{-4}$	J kg^{-1} K^{-1}
r_{22}	$0.234\,801\,409\,215\,913 \times 10^{-10}$	$-0.285\,651\,142\,904\,972 \times 10^{-10}$	J kg^{-1} K^{-1}

This list of 18 parameters contains two redundant ones that formally appeared during the transformation of six real parameters describing heat capacity into four complex numbers, see Feistel and Wagner [6].

The complex logarithm $\ln(z)$ is meant as the principal value, i.e. it evaluates to imaginary parts in the interval $-\pi < \mathrm{Im}\left[\ln(z)\right] \le +\pi$ (the number Pi, $\pi = 3.1415\ldots$, in this inequality is not to be confused with the symbol of reduced pressure). The complex notation used here has no direct physical basis but serves for convenience of analytical partial derivatives and for compactness of the resulting formulae, especially in program code. Complex data types are supported by scientific computer languages like Fortran (as COMPLEX*16) or C++ (as complex <double>), thus allowing an immediate implementation of the formulae given, without the need for prior conversion to much more complicated real functions, or for experience in complex calculus.

The residual entropy coefficient s_0 is given in Table 2 in the form of two alternative values. The 'IAPWS-95' value is required for phase equilibria studies between ice and fluid water in the IAPWS-95 formulation [2, 7], or seawater (Feistel [8]), while its 'absolute' alternative represents the true physical zero-point entropy of ice (Pauling [9], Nagle [10]).

'IAPWS-95' reference state [2, 7]:

$$u^{\mathrm{L}}\left(T_{\mathrm{t}}, p_{\mathrm{t}}^{\mathrm{num}}\right) = 0$$
$$s^{\mathrm{L}}\left(T_{\mathrm{t}}, p_{\mathrm{t}}^{\mathrm{num}}\right) = 0 \qquad (2)$$

'Absolute' reference state:

$$g\left(T = 0\ \mathrm{K}, p_0\right) = -0.632\ 020\ 233\ 335\ 886 \times 10^{6}\ \mathrm{J\,kg^{-1}}$$
$$s\left(T = 0\ \mathrm{K}, p_0\right) = 0.189\ 13 \times 10^{3}\ \mathrm{J\,kg^{-1}\,K^{-1}} \qquad (3)$$

The superscript 'L' indicates the liquid phase. The property u is the specific internal energy, see Table 3, Eq. (8). The theoretical absolute value for the internal energy is given by the relativistic rest energy, a very large number of the order of $10^{17}\ \mathrm{J\,kg^{-1}}$, which is too impractical to be adopted here. Thus, to conveniently specify g_{00}, the second free constant of the reference state defined by Eq. (3), the value of g at zero absolute temperature and normal pressure is chosen here for simplicity to be the same for both reference states.

TABLE 3 Relations of the thermodynamic properties to the equation for the Gibbs energy of ice, Eq. (1), and its derivatives[a]

Property	Relation	Unit	Eq.
Density			
$\rho(T,p) = v^{-1} = (\partial g/\partial p)_T^{-1}$	$\rho(T,p) = g_p^{-1}$	$\frac{\mathrm{kg}}{\mathrm{m}^3}$	(4)
Specific entropy			
$s(T,p) = -(\partial g/\partial T)_p$	$s(T,p) = -g_T$	$\frac{\mathrm{J}}{\mathrm{kg\ K}}$	(5)
Specific isobaric heat capacity			
$c_p(T,p) = T(\partial s/\partial T)_p$	$c_p(T,p) = -T g_{TT}$	$\frac{\mathrm{J}}{\mathrm{kg\ K}}$	(6)
Specific enthalpy			
$h(T,p) = g + Ts$	$h(T,p) = g - T g_T$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(7)
Specific internal energy			
$u(T,p) = g + Ts - pv$	$u(T,p) = g - T g_T - p g_p$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(8)
Specific Helmholtz energy			
$f(T,p) = g - pv$	$f(T,p) = g - p g_p$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(9)
Cubic expansion coefficient			
$\alpha(T,p) = v^{-1}(\partial v/\partial T)_p$	$\alpha(T,p) = g_{Tp}/g_p$	$\frac{1}{\mathrm{K}}$	(10)
Pressure coefficient			
$\beta(T,p) = (\partial p/\partial T)_v$	$\beta(T,p) = -g_{Tp}/g_{pp}$	$\frac{\mathrm{Pa}}{\mathrm{K}}$	(11)
Isothermal compressibility			
$\kappa_T(T,p) = -v^{-1}(\partial v/\partial p)_T$	$\kappa_T(T,p) = -g_{pp}/g_p$	$\frac{1}{\mathrm{Pa}}$	(12)
Isentropic compressibility			
$\kappa_s(T,p) = -v^{-1}(\partial v/\partial p)_s$	$\kappa_s(T,p) = \left(g_{Tp}^2 - g_{TT}\, g_{pp}\right)\big/\left(g_p\, g_{TT}\right)$	$\frac{1}{\mathrm{Pa}}$	(13)

[a] $g_T \equiv \left[\frac{\partial g}{\partial T}\right]_p$, $g_p \equiv \left[\frac{\partial g}{\partial p}\right]_T$, $g_{TT} \equiv \left[\frac{\partial^2 g}{\partial T^2}\right]_p$, $g_{Tp} \equiv \left[\frac{\partial^2 g}{\partial T \partial p}\right]$, $g_{pp} \equiv \left[\frac{\partial^2 g}{\partial p^2}\right]_T$

TABLE 4 Equations for the Gibbs energy of ice, Eq. (1), and its derivatives[a]

Equation for the Gibbs energy $g(T, p)$ and its derivatives[a]	Unit
$g(T,p) = g_0 - s_0 T_t\,\tau + T_t\,\mathrm{Re}\left(\sum_{k=1}^{2} r_k \left[(t_k-\tau)\ln(t_k-\tau) + (t_k+\tau)\ln(t_k+\tau) - 2t_k\ln(t_k) - \frac{\tau^2}{t_k}\right]\right)$	$\frac{\mathrm{J}}{\mathrm{kg}}$
with $\tau = T/T_t$, $\pi = p/p_t$, $T_t = 273.16\ \mathrm{K}$, $p_t = 611.657\ \mathrm{Pa}$, $g_0(p)$, $r_2(p)$	
$g_T = -s_0 + \mathrm{Re}\left(\sum_{k=1}^{2} r_k \left[-\ln(t_k-\tau) + \ln(t_k+\tau) - 2\frac{\tau}{t_k}\right]\right)$	$\frac{\mathrm{J}}{\mathrm{kg\ K}}$
$g_p = g_{0,p} + T_t\,\mathrm{Re}\left(r_{2,p}\left[(t_2-\tau)\ln(t_2-\tau) + (t_2+\tau)\ln(t_2+\tau) - 2t_2\ln(t_2) - \frac{\tau^2}{t_2}\right]\right)$	$\frac{\mathrm{m}^3}{\mathrm{kg}}$
$g_{TT} = \frac{1}{T_t}\mathrm{Re}\left(\sum_{k=1}^{2} r_k \left[\frac{1}{t_k-\tau} + \frac{1}{t_k+\tau} - \frac{2}{t_k}\right]\right)$	$\frac{\mathrm{J}}{\mathrm{kg\ K^2}}$
$g_{Tp} = \mathrm{Re}\left(r_{2,p}\left[-\ln(t_2-\tau) + \ln(t_2+\tau) - 2\frac{\tau}{t_2}\right]\right)$	$\frac{\mathrm{m}^3}{\mathrm{kg\ K}}$
$g_{pp} = g_{0,pp} + T_t\,\mathrm{Re}\left(r_{2,pp}\left[(t_2-\tau)\ln(t_2-\tau) + (t_2+\tau)\ln(t_2+\tau) - 2t_2\ln(t_2) - \frac{\tau^2}{t_2}\right]\right)$	$\frac{\mathrm{m}^3}{\mathrm{kg\ Pa}}$

$g_0(p)$ equation and its derivatives[b]	Unit	$r_2(p)$ equation and its derivatives[b]	Unit
$g_0(p) = \sum_{k=0}^{4} g_{0k}(\pi-\pi_0)^k$	$\frac{\mathrm{J}}{\mathrm{kg}}$	$r_2(p) = \sum_{k=0}^{2} r_{2k}(\pi-\pi_0)^k$	$\frac{\mathrm{J}}{\mathrm{kg\ K}}$
with $\pi_0 = \frac{p_0}{p_t} = \frac{101\,325\ \mathrm{Pa}}{611.657\ \mathrm{Pa}}$		with $\pi_0 = \frac{p_0}{p_t} = \frac{101\,325\ \mathrm{Pa}}{611.657\ \mathrm{Pa}}$	
$g_{0,p} = \sum_{k=1}^{4} g_{0k}\frac{k}{p_t}(\pi-\pi_0)^{k-1}$	$\frac{\mathrm{m}^3}{\mathrm{kg}}$	$r_{2,p} = \sum_{k=1}^{2} r_{2k}\frac{k}{p_t}(\pi-\pi_0)^{k-1}$	$\frac{\mathrm{m}^3}{\mathrm{kg\ K}}$
$g_{0,pp} = \sum_{k=2}^{4} g_{0k}\frac{k(k-1)}{p_t^2}(\pi-\pi_0)^{k-2}$	$\frac{\mathrm{m}^3}{\mathrm{kg\ Pa}}$	$r_{2,pp} = r_{22}\frac{2}{p_t^2}$	$\frac{\mathrm{m}^3}{\mathrm{kg\ Pa\ K}}$

[a] $g_T \equiv \left[\frac{\partial g}{\partial T}\right]_p$, $g_p \equiv \left[\frac{\partial g}{\partial p}\right]_T$, $g_{TT} \equiv \left[\frac{\partial^2 g}{\partial T^2}\right]_p$, $g_{Tp} \equiv \left[\frac{\partial^2 g}{\partial T\,\partial p}\right]$, $g_{pp} \equiv \left[\frac{\partial^2 g}{\partial p^2}\right]_T$

[b] $g_{0,p} \equiv \left[\frac{\partial g_0}{\partial p}\right]_T$, $g_{0,pp} \equiv \left[\frac{\partial^2 g_0}{\partial p^2}\right]_T$, $r_{2,p} \equiv \left[\frac{\partial r_2}{\partial p}\right]_T$, $r_{2,pp} \equiv \left[\frac{\partial^2 r_2}{\partial p^2}\right]_T$

4 Relations of the Thermodynamic Properties to the Specific Gibbs Energy

Thermodynamic properties can be derived from Eq. (1) by using the appropriate combinations of the specific Gibbs energy and its derivatives. Relations between thermodynamic properties and $g(T,p)$ and its derivatives are summarized in Table 3. All required derivatives of the specific Gibbs energy are explicitly given in Table 4.

5 Range of Validity and Brief Discussion

The equation of state, Eq. (1), is valid in the entire existence region of naturally abundant, hexagonal ice Ih of H_2O, covering the temperature and pressure range

$$0\ \mathrm{K} \le T \le 273.16\ \mathrm{K} \quad \text{and} \quad 0 \le p \le 210\ \mathrm{MPa},$$

see Fig. 1. The temperatures are based on the temperature scale ITS-90. The evaluation of the phase-equilibrium condition between ice and liquid water ($g = g^{\mathrm{L}}$ with g calculated from Eq. (1) and g^{L} calculated from IAPWS-95 [7]) and between ice and water vapor ($g = g^{\mathrm{V}}$ with g calculated from Eq. (1) and g^{V} calculated from IAPWS-95 [7]) allows a thermodynamically consistent computation of the melting-pressure and sublimation-pressure curves, being improved especially near the triple point, and valid down to 130 K sublimation temperature. In this way, for example, a value for the melting temperature at the normal pressure p_0 could be determined, namely T_{melt,p_0} = 273.152 519 K with an estimated uncertainty of only 2 µK [1], see the footnote of Table 5. IAPWS-95 only yields reliable vapor heat capacities down to 130 K; the calculation of the sublimation-pressure curve to temperatures below this limit is possible with a suitable extension [11, 12].

Information on the experimental data of ice Ih used to develop the equation of state, Eq. (1), is given in [1].

The theoretical formalism of classical thermodynamics is, in the strict sense, only valid for equilibrium states. For the case of ice, this means that the potential function is designed to describe the ideal structure of a single, undistorted crystal at a state where all possible spontaneous aging processes have passed. These conditions may not always be fulfilled exactly for the experimental data used. Especially in the temperature range below 100 K, the related theoretical and experimental problems are complicated and still subject to ongoing research. Excessive scatter is observed in measurements of heat capacity and density in the range between 60 K and 100 K. Results of different works deviate from each other more (up to 0.3% in density) than their particular precisions suggest, so that systematic problems in sample preparations or experimental procedures must be inferred [13-16]. The Gibbs function presented in this paper ignores the various open questions in the low-temperature region and treats ice Ih like a stable equilibrium phase down to 0 K. The majority of the various measured thermodynamic equilibrium properties are described by the equation of state, Eq. (1), within their experimental uncertainties [1].

Close to zero temperature, Eq. (1) obeys the theoretical cubic limiting law of Debye for heat capacity and the Third Law by Pauling's pressure-independent residual entropy.

Note: Consistent with this Release, IAPWS has issued the Revised Release on the *Pressure along the Melting and Sublimation Curves of Ordinary Water Substance* [12] containing a set of simple correlation equations which yield values for the melting and the sublimation pressure of ice Ih.

6 Estimates of Uncertainty

Combined standard uncertainties u_c reported in the following, estimated directly or indirectly from experimental data, were obtained during the numerical construction of the equation of state and exploiting its inherent consistency. Here, estimated combined standard uncertainties u_c [17] are reported, from which expanded uncertainties $U = k\,u_c$ can be obtained by multiplying with the coverage factor $k = 2$, corresponding to a 95% level of confidence. The term 'uncertainty' used in the following refers to combined standard uncertainties or to relative combined standard uncertainties.

TABLE 5 Summary of estimated combined standard uncertainties of selected quantities in certain regions of the *T*-*p* space, derived from corresponding experiments

Quantity	*T* interval	*p* interval	Uncertainty
$u_c(g)$	$T \le 273$ K	$p \le 0.1$ MPa	$2\ \mathrm{J\,kg^{-1}\,K^{-1}} \times \lvert T - T_t \rvert$
$u_c(g)$	238 K $\le T \le$ 273 K	$p \le 200$ MPa	$2\ \mathrm{J\,kg^{-1}\,K^{-1}} \times \lvert T - T_t \rvert + 2 \times 10^{-6}\ \mathrm{J\,kg^{-1}\,Pa^{-1}} \times \lvert p - p_t \rvert$
$u_c(h)$	$T \le 273$ K	$p \le 0.1$ MPa	$600\ \mathrm{J\,kg^{-1}}$
$u_c(\Delta h_{melt})$	$T = 273.15$ K	$p = 0.1$ MPa	$200\ \mathrm{J\,kg^{-1}}$
$u_c(\Delta h_{subl})$	130 K $\le T \le$ 273 K	100 nPa $\le p$	$4\ \mathrm{J\,kg^{-1}\,K^{-1}} \times T$
$u_c(\mathrm{d}p_{melt}/\mathrm{d}T)$	$T = 273.15$ K	$p = 0.1$ MPa	$3 \times 10^3\ \mathrm{Pa\,K^{-1}}$
$u_c(T_{melt})$	273.15 K $\le T$	$p \le 0.1$ MPa	2×10^{-6} K[a]
$u_c(T_{melt})$	273.11 K $\le T$	$p \le 0.6$ MPa	40×10^{-6} K
$u_c(T_{melt})$	266 K $\le T \le$ 273 K	$p \le 100$ MPa	$2 \times 10^{-9}\ \mathrm{K\,Pa^{-1}} \times p$
$u_c(T_{melt})$	259 K $\le T \le$ 266 K	100 MPa $\le p \le$ 150 MPa	0.5 K
$u_c(p_{melt}) / p_{melt}$	266 K $\le T \le$ 273 K	$p \le 100$ MPa	2 %
$u_c(p_{subl})$	257 K $\le T \le$ 273 K	100 Pa $\le p$	0.4 Pa
$u_c(p_{subl}) / p_{subl}$	130 K $\le T \le$ 257 K	100 nPa $\le p \le$ 100 Pa	0.6 %
$u_c(s)$	$T \le 273$ K	$p \le 0.1$ MPa	$2\ \mathrm{J\,kg^{-1}\,K^{-1}}$
$u_c(c_p) / c_p$	$T \le 273$ K	$p \le 0.1$ MPa	2 %
$u_c(\rho) / \rho$	268 K $\le T \le$ 273 K	$p \le 0.1$ MPa	0.02 %
$u_c(\rho) / \rho$	$T \le 268$ K	$p \le 0.1$ MPa	0.1 %
$u_c(\rho) / \rho$	238 K $\le T \le$ 273 K	$p \le 200$ MPa	0.2 %
$u_c(\alpha)$	243 K $\le T \le$ 273 K	$p \le 0.1$ MPa	$2 \times 10^{-6}\ \mathrm{K^{-1}}$
$u_c(\alpha)$	100 K $\le T \le$ 243 K	$p \le 0.1$ MPa	$5 \times 10^{-6}\ \mathrm{K^{-1}}$
$u_c(\kappa_s)$, $u_c(\kappa_T)$	60 K $\le T \le$ 273 K	$p \le 0.1$ MPa	$1 \times 10^{-12}\ \mathrm{Pa^{-1}}$
$u_c(\kappa_s)$, $u_c(\kappa_T)$	238 K $\le T \le$ 273 K	$p \le 200$ MPa	$1 \times 10^{-12}\ \mathrm{Pa^{-1}}$

[a] This value is based on an exact triple-point temperature. If isotopic fractionation is accounted for, the additional uncertainty of the triple-point temperature of 14 μK must be included [2].

The fundamental information about the uncertainty of a particular quantity in a certain region of the *T-p* space is adopted from the uncertainties reported or estimated for the most accurate related experimental data. If such uncertainties were unavailable or inappropriate, our estimates were based on the quantitative agreement and consistency of the data considered, with respect to the present formulation. For cases without any corresponding measurements, attempts were made to derive the required uncertainties from other, measured parameters using thermodynamic rules. Especially for these quantities, more detailed derivations are given in the article by Feistel and Wagner [1].

A summary of estimated combined standard uncertainties of selected quantities in certain regions of the *T-p* space is given in Table 5. The uncertainty of density in different regions of the *T-p* space is shown in Fig. 1.

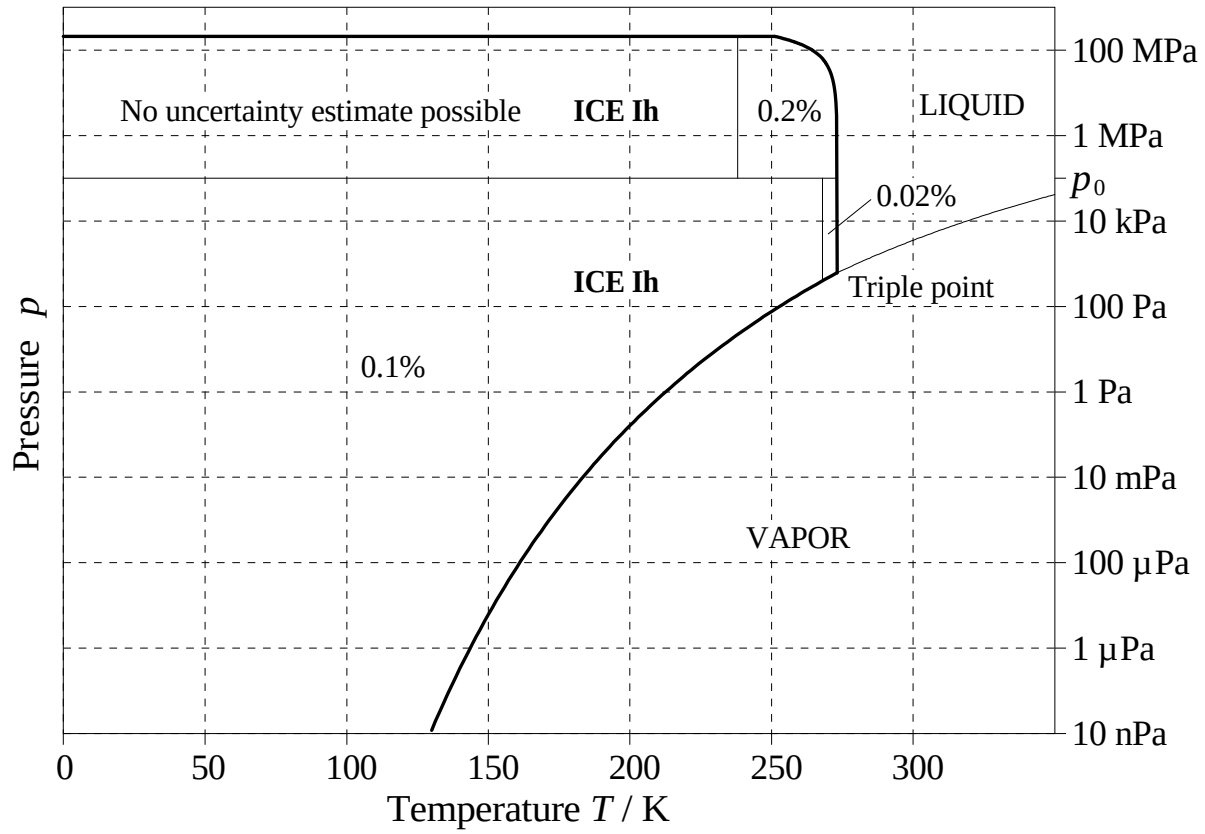

Fig. 1 Relative combined standard uncertainty of ice density, $u_c(\rho)/\rho$, Table 5, estimated for different regions of the *T-p* space. No experimental high-pressure data are available at low temperatures. This figure also illustrates the range of validity of the equation of state, Eq. (1).

7 Computer-Program Verification

To assist the user in computer-program verification, Table 6 with test values is given. It contains values for the specific Gibbs energy, $g(T,p)$, together with the corresponding derivatives and some thermodynamic properties.

8 References

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TABLE 6 Properties at the triple point, the normal pressure melting point, and at T = 100 K, p = 100 MPa, usable as numerical check values. The numerical functions evaluated here at given points (T, p) are defined in Eq. (1) and Tables 3 and 4, computed with the "IAPWS-95" value of s_0 from Table 2. The digits given in this table can reasonably be expected to be reproduced by rounded results from double-precision code [2]

Quantity	Value at $T = T_t = 273.16$ K $p = p_t = 611.657$ Pa	Value at $T = T_{melt,\, p_0} = 273.152\,519$ K $p = p_0 = 101\,325$ Pa	Value at T = 100 K p = 100 MPa	Unit
g	$0.611\,784\,135$	$0.101\,342\,740\,69 \times 10^{3}$	$-0.222\,296\,513\,088 \times 10^{6}$	J kg^{-1}
$(\partial g/\partial p)_T$	$0.109\,085\,812\,737 \times 10^{-2}$	$0.109\,084\,388\,214 \times 10^{-2}$	$0.106\,193\,389\,260 \times 10^{-2}$	m^3 kg^{-1}
$(\partial g/\partial T)_p$	$0.122\,069\,433\,940 \times 10^{4}$	$0.122\,076\,932\,550 \times 10^{4}$	$0.261\,195\,122\,589 \times 10^{4}$	J kg^{-1} K^{-1}
$(\partial^2 g/\partial p^2)_T$	$-0.128\,495\,941\,571 \times 10^{-12}$	$-0.128\,485\,364\,928 \times 10^{-12}$	$-0.941\,807\,981\,761 \times 10^{-13}$	m^3 kg^{-1} Pa^{-1}
$\partial^2 g/\partial p \partial T$	$0.174\,387\,964\,700 \times 10^{-6}$	$0.174\,362\,219\,972 \times 10^{-6}$	$0.274\,505\,162\,488 \times 10^{-7}$	m^3 kg^{-1} K^{-1}
$(\partial^2 g/\partial T^2)_p$	$-0.767\,602\,985\,875 \times 10$	$-0.767\,598\,233\,365 \times 10$	$-0.866\,333\,195\,517 \times 10$	J kg^{-1} K^{-2}
h	$-0.333\,444\,253\,966 \times 10^{6}$	$-0.333\,354\,873\,637 \times 10^{6}$	$-0.483\,491\,635\,676 \times 10^{6}$	J kg^{-1}
f	$-0.554\,468\,75 \times 10^{-1}$	$-0.918\,701\,567 \times 10$	$-0.328\,489\,902\,347 \times 10^{6}$	J kg^{-1}
u	$-0.333\,444\,921\,197 \times 10^{6}$	$-0.333\,465\,403\,393 \times 10^{6}$	$-0.589\,685\,024\,936 \times 10^{6}$	J kg^{-1}
s	$-0.122\,069\,433\,940 \times 10^{4}$	$-0.122\,076\,932\,550 \times 10^{4}$	$-0.261\,195\,122\,589 \times 10^{4}$	J kg^{-1} K^{-1}
c_p	$0.209\,678\,431\,622 \times 10^{4}$	$0.209\,671\,391\,024 \times 10^{4}$	$0.866\,333\,195\,517 \times 10^{3}$	J kg^{-1} K^{-1}
ρ	$0.916\,709\,492\,200 \times 10^{3}$	$0.916\,721\,463\,419 \times 10^{3}$	$0.941\,678\,203\,297 \times 10^{3}$	kg m^{-3}
α	$0.159\,863\,102\,566 \times 10^{-3}$	$0.159\,841\,589\,458 \times 10^{-3}$	$0.258\,495\,528\,207 \times 10^{-4}$	K^{-1}
β	$0.135\,714\,764\,659 \times 10^{7}$	$0.135\,705\,899\,321 \times 10^{7}$	$0.291\,466\,166\,994 \times 10^{6}$	Pa K^{-1}
κ_T	$0.117\,793\,449\,348 \times 10^{-9}$	$0.117\,785\,291\,765 \times 10^{-9}$	$0.886\,880\,048\,115 \times 10^{-10}$	Pa^{-1}
κ_s	$0.114\,161\,597\,779 \times 10^{-9}$	$0.114\,154\,442\,556 \times 10^{-9}$	$0.886\,060\,982\,687 \times 10^{-10}$	Pa^{-1}