

The International Association for the Properties of Water and Steam

Plzeň, Czech Republic

September 2011

Revised Supplementary Release on Properties of Liquid Water at 0.1 MPa

© 2011 International Association for the Properties of Water and Steam

Publication in whole or in part is allowed in all countries provided that attribution is given to the International Association for the Properties of Water and Steam

President:

Karol Daucik

Larok s.r.o.

SK-96263 Pliesovce, Slovakia

Executive Secretary:

Dr. R. B. Dooley

Structural Integrity Associates, Inc.

2616 Chelsea Drive

Charlotte, NC 28209, USA

email: bdooley@structint.com

This supplementary release is a revision of the corresponding supplementary release of 2008.

It contains 12 pages, including this cover page.

This supplementary release has been authorized by the International Association for the Properties of Water and Steam (IAPWS) at its meeting in Plzeň, Czech Republic, 4-9 September 2011, for issue by its Secretariat. The members of IAPWS are: Britain and Ireland, Canada, the Czech Republic, Germany, Japan, Russia, Scandinavia (Denmark, Finland, Norway, Sweden), and the United States of America, and associate members Argentina and Brazil, Australia, France, Greece, Italy, New Zealand, and Switzerland.

The correlations in this document are identical to the “Supplementary Release on Properties of Liquid Water at 0.1 MPa” adopted in 2008, except that the correlation for the thermal conductivity has been updated to correspond to the 2011 IAPWS release for that property.

Further information concerning this supplementary release and other documents issued by IAPWS can be obtained from the Executive Secretary of IAPWS or from <http://www.iapws.org>.

Contents

1.	Introductory Remarks	2
2.	Thermodynamic Properties	2
2.1	Basis for correlation	2
2.2	Correlating equations	2
2.3	Range of applicability and uncertainty	4
2.4	Application at standard atmospheric pressure	6
2.5	Application in a limited pressure range	6
3.	Viscosity	8
3.1	Basis for correlation	8
3.2	Correlating equation	8
3.3	Range of applicability and uncertainty	8
4.	Thermal Conductivity	8
4.1	Basis for correlation	8
4.2	Correlating equation	9
4.3	Range of applicability and uncertainty	9
5.	Static Dielectric Constant	9
5.1	Basis for correlation	9
5.2	Correlating equation	9
5.3	Range of applicability and uncertainty	10
6.	Calculations at Other Pressures	10
7.	Computer-Program Verification	10
8.	References	11

1. Introductory Remarks

This supplementary release provides correlating equations for various thermophysical properties of liquid water as a function of absolute temperature T at a standard pressure of 0.1 MPa. The purpose of these equations is to provide a convenient representation of these properties at this common condition, with uncertainties no greater than those of the more complex IAPWS formulations that cover wide ranges of temperature and pressure. A discussion of the background, development, and validation of these correlations is presented in Ref. [1]. The thermal conductivity correlation given in Ref. [1] has been superseded by the correlation given in Sec. 4 as documented in Ref. [8].

Section 2 of this supplementary release describes the calculation of thermodynamic properties, along with the range of applicability and uncertainty of the calculations. Similar information is provided for the viscosity in Section 3, for the thermal conductivity in Section 4, and for the static dielectric constant in Section 5. Section 6 discusses use of these correlations for liquid water at pressures differing from 0.1 MPa. Section 7 presents calculated values for computer-program verification.

2. Thermodynamic Properties

2.1. Basis for correlation

This correlation is designed to approximate closely values calculated from the IAPWS Formulation 1995 for the Thermodynamic Properties of Ordinary Water Substance for General and Scientific Use [2,3].

2.2. Correlating equations

Thermodynamic properties of liquid water at a pressure $p_0 = 0.1$ MPa are correlated by equations for specific Gibbs energy g , specific volume v , and isothermal derivative of specific volume with respect to pressure $v_p \equiv (\partial v / \partial p)_T$:

$$g_0 \equiv g(p_0, T) = RT_R \left(c_1 + c_2 \tau + c_3 \tau \ln \tau + \sum_{i=1}^3 a_i \alpha^{n_i} + \sum_{i=1}^4 b_i \beta^{m_i} \right), \quad (1)$$

$$v_0 \equiv v(p_0, T) = \frac{RT_R}{p_0} \left(a_5 + \sum_{i=6}^{10} a_i \alpha^{n_i} + \sum_{i=5}^{10} b_i \beta^{m_i} \right), \quad (2)$$

$$v_{p0} \equiv v_p(p_0, T) = \frac{RT_R}{p_0^2} \left(\sum_{i=11}^{15} a_i \alpha^{n_i} + \sum_{i=11}^{17} b_i \beta^{m_i} \right), \quad (3)$$

where $R = 461.51805 \text{ J} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$, $T_R = 10 \text{ K}$, and dimensionless coefficients a_i , b_i and c_i , and exponents n_i and m_i , are given in Table 1. Quantities τ , α and β are given as

$$\tau = \frac{T}{T_R}, \quad \alpha = \frac{T_R}{T_a - T}, \quad \beta = \frac{T_R}{T - T_b}, \quad (4)$$

where T is temperature in K, $T_a = 593 \text{ K}$, and $T_b = 232 \text{ K}$.

Further thermodynamic properties are derived from Eqs. (1)-(3) using thermodynamic identities. Quantities obtained by differentiating Eqs. (1)-(3) are given in Table 2. Table 3 shows relations for properties obtained by algebraic combinations of quantities given by Eqs. (1)-(3) and quantities given in Table 2.

Table 1. Coefficients and exponents of Eqs. (1)-(3)

Eq.	i	n_i	m_i	a_i	b_i	c_i
(1)	1	4	2	$-1.661470539\text{E}+5$	$-8.237426256\text{E}-1$	$-2.452093414\text{E}+2$
	2	5	3	$2.708781640\text{E}+6$	1.908956353	$3.869269598\text{E}+1$
	3	7	4	$-1.557191544\text{E}+8$	-2.017597384	-8.983025854
	4	n/a	5	n/a	$8.546361348\text{E}-1$	
(2)	5	n/a	1	$1.93763157\text{E}-2$	$5.78545292\text{E}-3$	
	6	4	2	$6.74458446\text{E}+3$	$-1.53195665\text{E}-2$	
	7	5	3	$-2.22521604\text{E}+5$	$3.11337859\text{E}-2$	
	8	7	4	$1.00231247\text{E}+8$	$-4.23546241\text{E}-2$	
	9	8	5	$-1.63552118\text{E}+9$	$3.38713507\text{E}-2$	
	10	9	6	$8.32299658\text{E}+9$	$-1.19946761\text{E}-2$	
(3)	11	1	1	$-7.5245878\text{E}-6$	$-3.1091470\text{E}-6$	
	12	3	3	$-1.3767418\text{E}-2$	$2.8964919\text{E}-5$	
	13	5	4	$1.0627293\text{E}+1$	$-1.3112763\text{E}-4$	
	14	6	5	$-2.0457795\text{E}+2$	$3.0410453\text{E}-4$	
	15	7	6	$1.2037414\text{E}+3$	$-3.9034594\text{E}-4$	
	16		7		$2.3403117\text{E}-4$	
	17		9		$-4.8510101\text{E}-5$	

NOTE: The notation $y\text{E}\pm n$ in Table 1 should be interpreted as $y \times 10^{\pm n}$.

2.3. Range of applicability and uncertainty

The correlation of thermodynamic properties at $p_0 = 0.1$ MPa given by Eqs. (1)-(3) is recommended for use in the following temperature range:

$$253.15 \text{ K} \leq T \leq 383.15 \text{ K}. \quad (5)$$

It should not be extrapolated outside these limits. At some temperatures within this range, the equilibrium phase at 0.1 MPa is a solid (below approximately 273.15 K) or a vapor (above approximately 372.76 K); at these conditions Eqs. (1)-(3) describe the properties of the metastable liquid phase.

The uncertainty of Eqs. (1)-(3) (which can be considered as an estimate of the standard uncertainty with coverage factor $k=2$) is that of the underlying IAPWS Formulation [2,3]. In the stable region, this is a relative uncertainty of 0.0001 % for specific volume (or density), 0.005 % for the speed of sound, and 0.1 % for specific isobaric heat capacity. No uncertainty estimate is given for the metastable regions, but the agreement with available data for the subcooled region is within about 0.01 % in density, 1 % in speed of sound, and 1 % in isobaric heat capacity.

The mathematical structure of Eqs. (1)-(3) corresponds to the fact that the underlying IAPWS Formulation 1995 shows two singular points at 0.1 MPa, one below the freezing point, and one above the boiling point. The present correlation has singular points at $T = T_a$ and $T = T_b$. These singular points lie outside the range of validity of the present correlation. The values of T_a and T_b have no physical significance.

Table 2. Thermodynamic properties of liquid water at 0.1 MPa obtained by differentiating Eqs. (1)-(3):

Property	Relation
Specific entropy	
[derived from Eq. (1)]	$s_0 = -\frac{dg_0}{dT} = -R \left[c_2 + c_3(1 + \ln \tau) + \sum_{i=1}^3 n_i a_i \alpha^{n_i+1} - \sum_{i=1}^4 m_i b_i \beta^{m_i+1} \right]$
Specific isobaric heat capacity	
[derived from Eq. (1)]	$c_{p0} = -T \frac{d^2 g_0}{dT^2}$ $= -R \left[c_3 + \tau \sum_{i=1}^3 n_i (n_i + 1) a_i \alpha^{n_i+2} + \tau \sum_{i=1}^4 m_i (m_i + 1) b_i \beta^{m_i+2} \right]$
$v_T \equiv (\partial v / \partial T)_p$	
[derived from Eq. (2)]	$v_{T0} = \frac{dv_0}{dT} = \frac{R}{p_0} \left(\sum_{i=6}^{10} n_i a_i \alpha^{n_i+1} - \sum_{i=5}^{10} m_i b_i \beta^{m_i+1} \right)$
* $v_{TT} \equiv (\partial^2 v / \partial T^2)_p$	
[derived from Eq. (2)]	$v_{TT0} = \frac{d^2 v_0}{dT^2} = \frac{R}{p_0 T_R} \left(\sum_{i=6}^{10} n_i (n_i + 1) a_i \alpha^{n_i+2} + \sum_{i=5}^{10} m_i (m_i + 1) b_i \beta^{m_i+2} \right)$
* $v_{pT} \equiv \partial^2 v / \partial p \partial T$	
[derived from Eq. (3)]	$v_{pT0} = \frac{dv_{p0}}{dT} = \frac{R}{p_0^2} \left(\sum_{i=11}^{15} n_i a_i \alpha^{n_i+1} - \sum_{i=11}^{17} m_i b_i \beta^{m_i+1} \right)$

* Derivatives v_{TT0} and v_{pT0} are only needed for computing thermodynamic properties at pressures different from 0.1 MPa (Table 4).

Table 3. Thermodynamic properties of liquid water at pressure 0.1 MPa given by algebraic combinations of Eqs. (1)-(3) and their derivatives.

Property	Relation	
Specific enthalpy	$h_0 = g_0 + Ts_0$	
Specific internal energy	$u_0 = g_0 + Ts_0 - p_0 v_0$	
Specific Helmholtz energy	$f_0 = g_0 - p_0 v_0$	
Specific isochoric heat capacity	$c_{v0} = c_{p0} + T v_{T0}^2 / v_{p0}$	
Isothermal compressibility	$\kappa_T \equiv -\frac{1}{v} \left(\frac{\partial v}{\partial p} \right)_T$	$\kappa_{T0} = -v_{p0} / v_0$
Thermal expansivity	$\alpha \equiv \frac{1}{v} \left(\frac{\partial v}{\partial T} \right)_p$	$\alpha_0 = v_{T0} / v_0$
Isentropic compressibility	$\kappa_s \equiv -\frac{1}{v} \left(\frac{\partial v}{\partial p} \right)_s$	$\kappa_{s0} = -\left(T v_{T0}^2 / c_{p0} + v_{p0} \right) / v_0$
Speed of sound	$w_0 = \left[-v_0^2 / \left(v_{p0} + T v_{T0}^2 / c_{p0} \right) \right]^{1/2}$	

2.4. Application at standard atmospheric pressure

The specific volume of liquid water at standard atmospheric pressure (defined as $p_{\text{atm}} = 0.101\,325$ MPa), computed as

$$v_{\text{atm}} = v_0 + v_{p0}(p_{\text{atm}} - p_0), \quad (6)$$

agrees in relative terms within 0.04×10^{-6} with the IAPWS Formulation 1995 [2,3] in the whole temperature interval given by Eq. (5). The speed of sound and specific isobaric heat capacity at standard atmospheric pressure can be taken equal to their values at 0.1 MPa, w_0 and c_{p0} , respectively, without an appreciable effect on the uncertainty.

2.5. Application in a limited pressure range

Relations for computing the thermodynamic properties of liquid water at pressures different from 0.1 MPa are given in Table 4. The uncertainties of the properties are essentially identical with the uncertainties of the IAPWS Formulation 1995 [2,3] in the pressure range from the vapor-liquid saturation pressure up to 0.3 MPa.

Table 4. Relations for thermodynamic properties of liquid water at pressure p different from 0.1 MPa.

Property	Relation
Specific Gibbs energy	$g \approx g_0 + v_0(p - p_0)$
Specific entropy	$s \approx s_0 - v_{T0}(p - p_0)$
Specific isobaric heat capacity	$c_p \approx c_{p0} - T v_{TT0}(p - p_0)$
Specific volume	$v \approx v_0 + v_{p0}(p - p_0)$
$v_T \equiv (\partial v / \partial T)_p$	$v_T \approx v_{T0} + v_{pT0}(p - p_0)$
$v_p \equiv (\partial v / \partial p)_T$	$v_p \approx v_{p0} + v_{pp0}(p - p_0)$
	where $v_{pp0} \equiv 3.24 \times 10^{-10} R T_R / p_0^3$
Specific enthalpy	$h = g + Ts$
Specific internal energy	$u = g + Ts - pv$
Specific Helmholtz energy	$f = g - pv$
Specific isochoric heat capacity	$c_v = c_p + T v_T^2 / v_p$
Isothermal compressibility	$\kappa_T = -v_p / v$
Thermal expansivity	$\alpha = v_T / v$
Isentropic compressibility	$\kappa_s = -(T v_T^2 / c_p + v_p) / v$
Speed of sound	$w = \left[-v^2 / (v_p + T v_T^2 / c_p) \right]^{1/2}$

3. Viscosity

3.1. Basis for correlation

This correlation is designed to approximate closely values calculated from the IAPWS Formulation 2008 for the Viscosity of Ordinary Water Substance [4,5].

3.2. Correlating equation

The viscosity μ of liquid water at a pressure of 0.1 MPa is described by the following equation:

$$\mu / (10^{-6} \text{ Pa} \cdot \text{s}) = \sum_{i=1}^4 a_i (T^*)^{b_i}, \quad (7)$$

where $T^* = T / (300 \text{ K})$ and the coefficients and exponents a_i and b_i are given in Table 5.

Table 5. Coefficients a_i and b_i for Eq. (7)

i	a_i	b_i
1	280.68	-1.9
2	511.45	-7.7
3	61.131	-19.6
4	0.459 03	-40.0

3.3. Range of applicability and uncertainty

Equation (7) is recommended for use in the following temperature range:

$$253.15 \text{ K} \leq T \leq 383.15 \text{ K}.$$

It should not be extrapolated outside these limits. At some temperatures within this range, the equilibrium phase at 0.1 MPa is a solid (below approximately 273.15 K) or a vapor (above approximately 372.76 K); at these conditions Eq. (7) describes the viscosity of the metastable liquid phase.

The uncertainty of Eq. (7) (which can be considered as an estimate of the standard uncertainty with coverage factor $k=2$) is that of the underlying IAPWS formulation [4,5]. This is 1 % for the stable liquid region. No uncertainty estimate is given for the metastable regions, but the agreement with available data for the subcooled region is within 5 %.

Equation (7) also reproduces the ISO recommended value of the viscosity at 20 °C (293.15 K) and standard atmospheric pressure within the number of digits given in Ref. [6]; it also agrees with all values from 288.15 to 313.15 K at atmospheric pressure in Ref. [6] within the stated uncertainty of 0.17 % at 293.15 K.

4. Thermal Conductivity

4.1. Basis for correlation

This correlation is designed to approximate closely values calculated from the IAPWS Formulation 2011 for the Thermal Conductivity of Ordinary Water Substance [7,8].

4.2. Correlating equation

The thermal conductivity λ of liquid water at a pressure of 0.1 MPa is described by the following equation:

$$\lambda / (1 \text{ W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}) = \sum_{i=1}^4 c_i (T^*)^{d_i}, \quad (8)$$

where $T^* = T / (300 \text{ K})$ and the coefficients and exponents c_i and d_i are given in Table 6.

Table 6. Coefficients c_i and d_i for Eq. (8)

i	c_i	d_i
1	1.663 0	-1.15
2	-1.778 1	-3.4
3	1.156 7	-6.0
4	-0.432 115	-7.6

4.3. Range of applicability and uncertainty

Equation (8) is recommended for use in the following temperature range:

$$273.15 \text{ K} \leq T \leq 383.15 \text{ K}.$$

In addition, it extrapolates in a physically realistic manner (matching the extrapolated behavior of the IAPWS Formulation; see Refs. [7] and [8] for discussion of this behavior) at temperatures down to 253.15 K. It should not be extrapolated outside these limits. At some temperatures within this range, the equilibrium phase at 0.1 MPa is a solid (below approximately 273.15 K) or a vapor (above approximately 372.76 K); at these conditions Eq. (8) describes the thermal conductivity of the metastable liquid phase.

The uncertainty of Eq. (8) (which can be considered as an estimate of the standard uncertainty with coverage factor $k=2$) is that of the underlying IAPWS formulation [7]. For the stable fluid region, this is given approximately by the uncertainty shown in Fig. 1 of the IAPWS release [7], which is 1.5 % in relative terms. No uncertainty is given for the thermal conductivity in metastable regions.

5. Static Dielectric Constant

5.1. Basis for correlation

In this case, some more accurate data for the liquid have become available since the IAPWS formulation [9,10] was adopted. Therefore, this correlation is designed to approximate values from Ref. [11] in the region above 273.15 K, and from Ref. [12] at subcooled liquid conditions. The treatment of these data is discussed in detail in Ref. [1].

5.2. Correlating equation

The static dielectric constant ε of liquid water at a pressure of 0.1 MPa is described by the following equation:

$$\varepsilon = \sum_{i=1}^4 e_i (T^*)^{f_i}, \quad (9)$$

where $T^* = T / (300 \text{ K})$ and the coefficients and exponents e_i and f_i are given in Table 7.

Table 7. Coefficients e_i and f_i for Eq. (9)

i	e_i	f_i
1	-43.7527	-0.05
2	299.504	-1.47
3	-399.364	-2.11
4	221.327	-2.31

5.3. Range of applicability and uncertainty

Equation (9) is recommended for use in the following temperature range:

$$253.15 \text{ K} \leq T \leq 383.15 \text{ K}.$$

It should not be extrapolated outside these limits. At some temperatures within this range, the equilibrium phase at 0.1 MPa is a solid (below approximately 273.15 K) or a vapor (above approximately 372.76 K); at these conditions Eq. (9) describes the dielectric constant of the metastable liquid phase.

The uncertainty of Eq. (9) (which can be considered as an estimate of the standard uncertainty with coverage factor $k=2$) is that of the underlying experimental data [11,12]. As discussed in [1], this is approximately 0.01 for the stable and superheated liquid region (above 273.15 K), but is much larger (approximately 1.0) for the subcooled liquid.

6. Calculations at Other Pressures

The formulations for viscosity, thermal conductivity, and static dielectric constant (Eqs. (7)-(9)) given here may be used for liquid water at any pressure between the vapor-liquid saturation pressure and 0.3 MPa without any significant loss in accuracy (meaning that the change in property due to the change in pressure is more than an order of magnitude smaller than the uncertainty of the property itself).

For some thermodynamic properties, additional calculations beyond the level of the basic Eqs. (1)-(3) may be necessary to maintain the required accuracy at pressures differing from 0.1 MPa. These calculations are described in Sections 2.4 and 2.5.

7. Computer-Program Verification

Table 8 is provided to assist the user in computer-program verification of Eqs. (1)-(3) [g_0 , v_0 , v_{p0}], Table 2 [s_0 , c_{p0} , v_{T0} , v_{TT0} , v_{pT0}], Eqs. (7)-(9) [μ , λ , ϵ], and the speed of sound w_0 as given in Table 3. Note that the number of digits printed in Table 8 greatly exceeds that justified by the uncertainty.

Table 8. Sample points for computer-program verification of calculated properties at 0.1 MPa.

Property	Units	Value at 260 K	Value at 298.15 K	Value at 375 K
Specific Gibbs energy, g_0	$\text{J}\cdot\text{kg}^{-1}$	-1265.9892	-4561.7537	-71 058.8021
Specific entropy, s_0	$\text{J}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}$	-209.985 55	367.201 45	1328.066 16
Specific isobaric Heat Capacity, c_{p0}	$\text{J}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}$	4300.174 72	4181.446 18	4217.746 97
Density, $\rho_0 = 1/v_0$	$\text{kg}\cdot\text{m}^{-3}$	997.068 360	997.047 013	957.009 710
Derivatives of v_0				
$10^7 v_{T0}$	$\text{m}^3\cdot\text{kg}^{-1}\cdot\text{K}^{-1}$	-3.865 509 41	2.580 54178	7.947 066 23
$10^8 v_{TT0}$	$\text{m}^3\cdot\text{kg}^{-1}\cdot\text{K}^{-2}$	3.274 425 03	0.972 020 76	0.620 241 04
$10^{13} v_{p0}$	$\text{m}^3\cdot\text{kg}^{-1}\cdot\text{Pa}^{-1}$	-5.820 968 20	-4.538 033 40	-5.156 665 28
$10^{15} v_{pT0}$	$\text{m}^3\cdot\text{kg}^{-1}\cdot\text{Pa}^{-1}\cdot\text{K}^{-1}$	7.809 382 94	1.000 385 67	-2.270 735 94
Speed of Sound, w_0	$\text{m}\cdot\text{s}^{-1}$	1324.872 58	1496.699 22	1541.466 11
Viscosity, μ	$\mu\text{Pa}\cdot\text{s}$	3058.360 75	889.996 774	276.207 245
Thermal Conductivity, λ	$\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$	0.515 628 010	0.606 502 308	0.677 913 788
Static Dielectric Constant, ε	(unitless)	93.455 835	78.375 218	55.266 199

8. References

- [1] Hrubý, J., Pátek, J., Klomfar, J., Součková, M., and Harvey, A. H., *J. Phys. Chem. Ref. Data* **38**, 21 (2009).
- [2] IAPWS, *Revised Release on the IAPWS Formulation 1995 for the Thermodynamic Properties of Ordinary Water Substance for General and Scientific Use*, available at <http://www.iapws.org> (2009).
- [3] Wagner, W., and Pruß, A., *J. Phys. Chem. Ref. Data* **31**, 387 (2002).
- [4] IAPWS, *Release on the IAPWS Formulation 2008 for the Viscosity of Ordinary Water Substance*, available at <http://www.iapws.org> (2008).
- [5] Huber, M. L., Perkins, R. A., Laesecke, A., Friend, D. G., Sengers, J. V., Assael, M. J., Metaxa, I. N., Vogel, E., Mareš, R., and Miyagawa, K., *J. Phys. Chem. Ref. Data* **38**, 101 (2009).
- [6] International Organization for Standardization (ISO), *Viscosity of Water*, ISO/TR Technical Report 3666: 1998(E), Geneva.
- [7] IAPWS, *Release on the IAPWS Formulation 2011 for the Thermal Conductivity of Ordinary Water Substance*, available at <http://www.iapws.org> (2011).

- [8] Huber, M. L., Perkins, R. A., Friend, D. G., Sengers, J. V., Assael, M. J., Metaxa, I. N., Miyagawa, K., Hellmann, R., and Vogel, E., *J. Phys. Chem. Ref. Data* **41**, 033102 (2012).
- [9] IAPWS, *Release on the Static Dielectric Constant of Ordinary Water Substance for Temperatures from 238 K to 873 K and Pressures up to 1000 MPa*, available at <http://www.iapws.org> (1997).
- [10] Fernández, D. P., Goodwin, A. R. H., Lemmon, E. W., Levelt Sengers, J. M. H., and Williams, R. C., *J. Phys. Chem. Ref. Data* **26**, 1125 (1997).
- [11] Hamelin, J., Mehl, J. B., and Moldover, M. R., *Int. J. Thermophys.* **19**, 1359 (1998).
- [12] Bertolini, D., Cassettari, M., and Salvetti, G., *J. Chem. Phys.* **76**, 3285 (1982).