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Static permittivity of water in electric field higher than $10^8 \, V \, m^{-1}$ and pressure varying from 0.1 to 600 MPa at room temperature

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A recently proposed statistical approach to the permittivity ε of water in the high electric field E (I. Danielewicz-Ferchmin, A.R. Ferchmin. *Phys. Chem. Chem. Phys*., **6**, 1332 (2004)) has been applied to water at $T = 293 \, K$ subjected to external pressure. Results are shown in the form of the set of isobars $\varepsilon(E)$, which reveal abrupt falls at $E \sim 10^9 \, V \, m^{-1}$.

1. Introduction

The aim of this work is to calculate the static permittivity ε of water in electric field $E > 10^8 \, V \, m^{-1}$ at pressures p in the range $0.1 < p < 600 \, MPa$ at room temperature. Electric fields higher than $10^8 \, V \, m^{-1}$ can be encountered in hydration layers arising when immersing charged surfaces with surface charge densities $\sigma_o \geq 9 \times 10^{-4} \, C \, m^{-2}$ in water. Such charge densities can exist, for example, at the surfaces of protein [1–3]. Characterization of protein surface hydration water is essential for understanding protein structure and folding [4]. It is generally known from experiment that proteins undergo denaturation when exposed to heating or sometimes cooling, to high pressure or too low and too high pH. Also, protein denaturation results from addition of denaturants [4]. For this reason, we have decided to calculate the permittivity ε of water in electric field higher than $10^8 \, V \, m^{-1}$ and under pressure varying from atmospheric to 600 MPa at $T = 293 \, K$. The knowledge of permittivity ε is necessary for developing further the research related to the phase diagram of electrostricted H_2O at enhanced external pressure. Since no relevant experimental data are available, calculation is the only way to obtain the knowledge about permittivity ε. The calculations are of interest since the results are expected to bring some information on the water response

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to high electric field under high pressure. This response needs to be regarded when studying the hydration shells of ions, of biomolecules or at charged electrodes with high external pressure applied.

2. Method

2.1. *A statistical model of water permittivity*

In this section, for the sake of completeness, some details of calculations appearing in the previous work [5] are re-derived in a form suitable for discussing the permittivity of water in the range of pressures $0.1 < p < 600\,\text{MPa}$ at room temperature. In this way, the method based on a statistical model of water permittivity proposed earlier has been extended so as to cope with the problem of the effect of external pressure variations. Application of the external pressure induces an increase in water density, which in turn leads to an increase in its permittivity ε. On the other hand, under applied pressure, up to values not exceeding 1 GPa, a part of hydrogen bonds is broken, which is reflected by an increase in the number I of allowed orientations of the dipole moments of water molecules.

2.2. *Linear approximation to the mean cosine*

To relate the electric permittivity ε to the dipole moment μ of a molecule one applies a statistical mechanical calculation leading to $\langle \cos\theta \rangle$ – the mean cosine [6] of the angle θ between the dipole moment μ of H_2O molecule and the field E. With no bounds imposed on the rotational motion of the dipole, it leads to the expression for $\langle \cos\theta \rangle$ in terms of the Langevin function [7,8] that provides correct predictions of the dielectric constant values for polar liquids with no hydrogen bonds. In this case, in the linear approximation,

$$\langle \cos\theta \rangle = \frac{\mu E_{\text{on}}}{3kT} \tag{1}$$

where E_{on} is the Onsager local field [6] and k denotes the Boltzmann constant. The above equation (1) for $\langle \cos\theta \rangle$ does not hold for liquids with hydrogen bonds [3,9,10]. For water, at ambient conditions, to achieve agreement with experiment, $\langle \cos\theta \rangle$ has been expressed [3,11] by a Brillouin function $B_2(\Xi)$ [7,8],

$$B_2(\Xi) = \tanh(\Xi), \tag{2}$$

$$\Xi = \frac{\mu E_{\text{on}}}{kT} \tag{3}$$

corresponding to only two allowed orientations of the dipole moment ($I = 2$) and then, in the linear approximation

$$\langle \cos\theta \rangle = \frac{\mu E_{\text{on}}}{kT} = \Xi. \tag{4}$$

The external electric field E is related to the Onsager local field E_{on} as follows ([6], equation 5.52, p. 175 therein):

$$E_{on} = \frac{\varepsilon(n^2 + 2)}{2\varepsilon + n^2} E,$$

(5)

where n denotes the refractive index. Note that both ε and n depend on pressure p. For the flat geometry of the space distribution of the charges generating the field E, we have

$$E = \frac{\sigma_0}{\varepsilon_0} = \frac{\sigma}{\varepsilon\varepsilon_0},$$

(6)

where σ is the total charge surface density and ε_0 is the permittivity of vacuum. Substituting equation (6) in equation (5) we get

$$E_{on} = \frac{n^2 + 2}{\varepsilon_0(2\varepsilon + n^2)} \sigma.$$

(7)

In the spherical geometry encountered around ions, E represents the Coulomb field

$$E = \frac{q}{4\pi\varepsilon\varepsilon_0 x^2},$$

(8)

where q is the elementary charge, x denotes reduced radius $x = r|Z|^{-1/2}$ (r, distance from the centre of the ion, Z, number of excess elementary charges of an ion) and we have

$$\sigma = \frac{q}{4\pi x^2}.$$

(9)

2.3. *Dielectric constant and Brillouin function in an approximation linear in the field E*

The value of $\langle\cos\theta\rangle$ for an arbitrary number I of allowed orientations of a dipole is expressed by the Brillouin function [7,8]

$$B_I(\Xi) = \frac{I}{I-1}\coth\frac{I\Xi}{I-1} - \frac{I}{I-1}\coth\frac{\Xi}{I-1},$$

(10)

where Ξ is defined in equation (3). For small values of the argument Ξ, the function $B_I(\Xi)$ can be expanded into the power series:

$$B_I(\Xi) = \frac{I+1}{3(I-1)}\Xi - \frac{I^4 - 1}{45(I-1)^4}\Xi^3 + \cdots \equiv b(I)\Xi - c(I)\Xi^3 + \cdots$$

(11)

Only the first term in the expansion, the linear term $b(I)\Xi$, is taken into account when one looks for the dielectric constant. The coefficient $b(I)$ and the mean number of orientations I of the dipole moment are interrelated as (cf. equation (11)):

$$b(I) = \frac{I+1}{3(I-1)}, \tag{12}$$

or inversely

$$I = \frac{3b+1}{3b-1}. \tag{13}$$

The relation between the permittivity ε and the electric field strength is, according to the Onsager field model [6], expressed as [3, 12]:

$$\frac{\varepsilon - n^2}{\varepsilon} = \frac{N^0 \mu(n^2 + 2)}{3\sigma v} \langle \cos\theta \rangle, \tag{14}$$

where v is the molar volume, N^0 is the Avogadro number,

$$\langle \cos\theta \rangle = B_I(\Xi), \tag{15}$$

for $I = 2$

$$\langle \cos\theta \rangle = \tanh(\Xi) \tag{16}$$

and from equations (3) and (7)

$$\Xi = \frac{\sigma\mu(n^2+2)}{kT\varepsilon_0(2\varepsilon + n^2)}. \tag{17}$$

The numerical value $b(I) = b(\infty) = 1/3$, in the theory of permittivity based on the Onsager model of local field E_{on} [6], follows from the assumption that all orientations of the dipoles are allowed and are equally probable ($I = \infty$) and one arrives at an expression for the dielectric constant ([6], p. 178, equation 5.67 therein):

$$\frac{3(\varepsilon - n^2)(2\varepsilon + n^2)}{\varepsilon(n^2 + 2)^2} = \frac{1}{3}\frac{\mu^2 N^0}{\varepsilon_0 vkT}, \tag{18}$$

where $b(\infty) = 1/3$. According to our proposed interpolation scheme, between the Langevin functions $L(\Xi)$, characteristic of most dipolar liquids, and hyperbolic tangent $\tanh(\Xi)$, characteristic of hydrogen-bonded liquids at ambient conditions [3,12], for small electric fields ($E \approx 10^3\,\mathrm{V\,m^{-1}}$), starting from the Brillouin function instead of the Langevin function, one arrives (equation (11)) at an analogous expression for the dielectric constant ε containing the factor $b(I)$ in place of $1/3$ present in equation (18):

$$\frac{3(\varepsilon - n^2)(2\varepsilon + n^2)}{\varepsilon(n^2 + 2)^2} = b(I)\frac{\mu^2 N^0}{\varepsilon_0 vkT}. \tag{19}$$

The numerical value of $b(I)$ can readily be found from equation (19) provided that the other quantities, and in particular the dielectric constant ε at a given temperature T and number density N^0/v (depending on pressure p), are known from the experiment. Note that $b(I)$ must satisfy the inequality:

$$\frac{1}{3} \leq b(I) \leq 1. \tag{20}$$

The empirical fact that the low-field dielectric constant data at atmospheric and higher pressures do indeed lead to the values for the coefficient $b(I)$ satisfying the inequality (20) confirms the possibility of application of our interpolation scheme. If the experimental data are such that $b(I)$ takes values leading to non-integer values of I (equation (13)), the function $B_I(\Xi)$ should be treated as defined by equation (10).

2.4. *Calculation of the permittivity* $\varepsilon = \varepsilon(p, T)$ *in fields* $E > 10^8\,V\,m^{-1}$ *and pressures not higher than 600 MPa*

Permittivity ε of water under pressure has been calculated on the basis of equation (14). Expressing $\langle \cos\theta \rangle$ in this equation by the function given by equation (10), this time without assuming the linear approximation in the field, we obtain

$$\frac{\varepsilon - n^2}{\varepsilon} = \frac{N^0 \mu (n^2 + 2)}{3\sigma v} \left[\frac{I}{I-1} \coth \frac{I\Xi}{I-1} - \frac{1}{I-1} \coth \frac{\Xi}{I-1} \right]. \tag{21}$$

The quantity Ξ given in equation (3), with the notation introduced in equation (5), can be written as

$$\Xi = \frac{\mu E}{kT} \frac{\varepsilon (n^2 + 2)}{2\varepsilon + n^2} \tag{22}$$

or, introducing the Coulomb field (equation (8)),

$$\Xi = \frac{q}{4\pi\varepsilon_0 x^2} \frac{\mu}{kT} \frac{(n^2 + 2)}{2\varepsilon + n^2}. \tag{23}$$

3. Results

Table 1 gives the physical quantities involved in equation (19) needed to find the values of $b(I)$. The second column of table 1 presents the values of the refractive index taken from literature [13] (for details see Appendix, table A1). The third column of table 1 shows the values of specific volumes of water [14] (Appendix, table A2). In the fourth column of the table, the values of the dielectric constant ε are given [15] (Appendix, table A3). The fifth and sixth columns display the calculated values of $b(I)$ and I, respectively, at room temperature and corresponding to the pressures

Table 1.   Values of the mean number I of allowed orientations of H_2O dipoles and other quantities entering equation (19) at room temperature and pressure from 0.1 to 600 MPa: n, refractive index [13], v, specific volume [14], ε, dielectric constant [15], coefficient $b(I)$, equation (12).

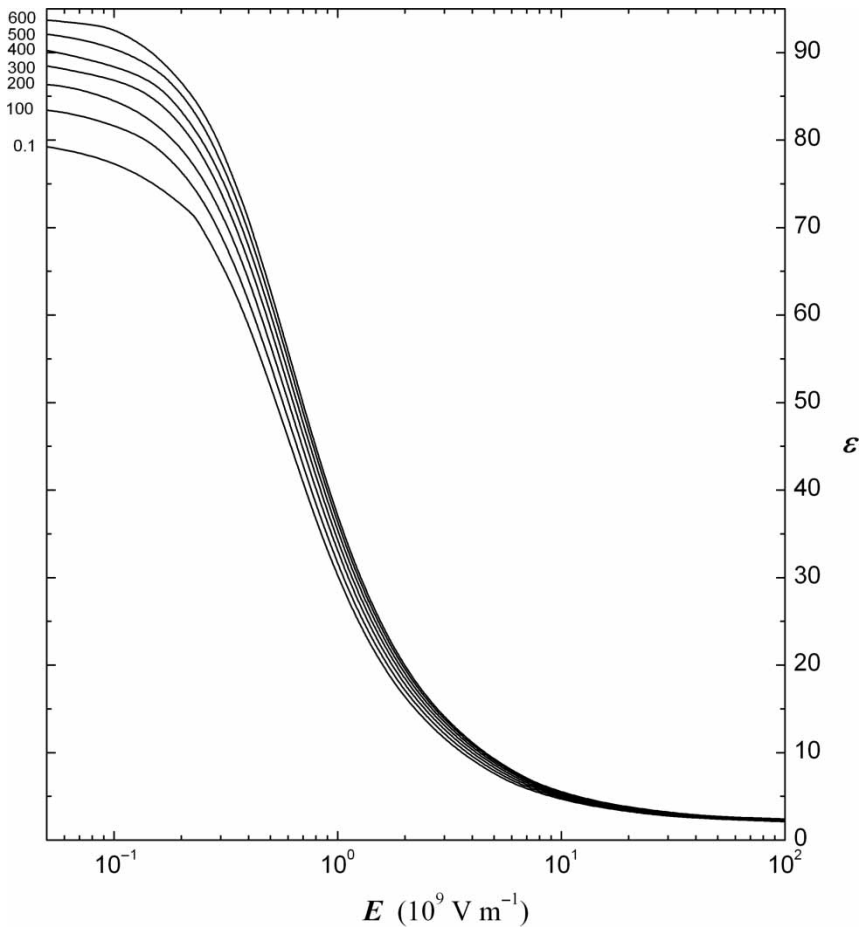| p (MPa)	n	v (cm^3 mol^{-1})	ε	$b(I)$	I
0.1	1.33311	18.0458	80.22	0.985	2.023
100	1.34365	17.3050	83.96	0.974	2.040
200	1.35349	16.6636	86.93	0.958	2.067
300	1.36299	16.1267	89.32	0.940	2.097
400	1.37230	15.6943	91.32	0.923	2.130
500	1.38139	15.3628	93.09	0.909	2.157
600	1.39003	15.1247	94.82	0.901	2.174

Figure 1.   Water permittivity $\varepsilon = \varepsilon(E)$ as a function of the field strength E under pressure from 0.1 to 600 MPa.
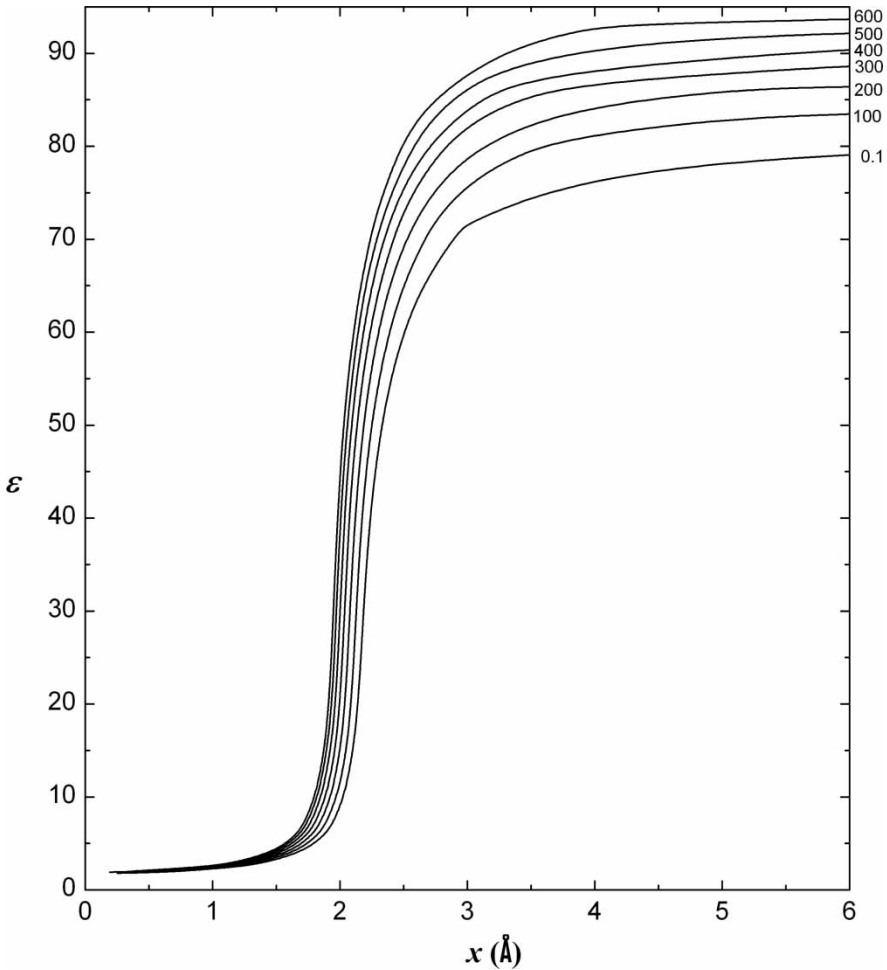
Figure 2. Water permittivity $\varepsilon = \varepsilon(x)$ as a function of the reduced distance x from the centre of an ion under pressure p from 0.1 to 600 MPa.

given in the first column. With these data at hand, our next task will be to calculate the permittivity ε in the high electric field and at high pressures p.

We have calculated the dependence of the permittivity ε on electric field strength, $\varepsilon = \varepsilon(E)$, on the basis of equation (21) with equation (22) taken into account. The dependence of the permittivity ε on the reduced distance from the centre of the ion x, $\varepsilon = \varepsilon(x)$ has been found on the basis of equation (21) with equation (23) taken into account. These results are shown in figures 1 and 2 as a set of isobars for pressures taken in the range $0.1 < p < 600$ MPa.

In both calculations the calculated permittivity ε is involved in the corresponding equations implicitly, i.e. on the left-hand side of the equation and on its right-hand side in the argument of the expression for $\langle \cos \theta \rangle$.

The results of these somewhat tedious calculations are presented in parallel in figures 1 and 2 and in tables 2–4. In these plots (figures 1 and 2), for small values of

E. Banachowicz and I. Danielewicz-Ferchmin

Table 2. Permittivity ε of water for electric field strength E or reduced radius x under pressures $p = 0.1$ MPa and $p = 100$ MPa calculated on the basis of equations (21)–(23).

$p = 0.1$ MPa			$p = 100$ MPa		
ε	x (Å)	$10^{-9}E$ (V m^{-1})	ε	x (Å)	$10^{-9}E$ (V m^{-1})
1.9	0.570	233.029	2	0.682	154.497
2	0.748	128.445	2.5	1.153	43.287
2.5	1.205	39.594	3	1.380	25.169
3	1.431	23.405	4	1.620	13.701
4	1.671	12.875	5	1.748	9.412
5	1.800	8.880	6	1.829	7.168
6	1.881	6.777	7	1.884	5.788
7	1.936	5.480	10	1.980	3.669
10	2.033	3.480	15	2.051	2.279
15	2.105	2.164	20	2.086	1.652
20	2.140	1.570	25	2.109	1.294
25	2.164	1.229	30	2.128	1.059
30	2.184	1.005	35	2.148	0.891
35	2.207	0.843	40	2.173	0.761
40	2.237	0.719	45	2.205	0.657
45	2.276	0.617	50	2.249	0.569
50	2.328	0.531	55	2.306	0.492
55	2.399	0.454	60	2.384	0.422
60	2.499	0.384	65	2.494	0.356
65	2.647	0.316	70	2.658	0.291
70	2.885	0.247	73	2.802	0.251
71	2.953	0.232	76	3.014	0.208
72	3.031	0.217	79	3.368	0.160
78	4.143	0.107	81	3.815	0.122
80	7.363	0.033	83	5.035	0.068
80.1	8.581	0.024	83.6	6.435	0.042
80.2	13.698	0.010	83.9	10.189	0.017

$E < 10^8$ V m^{-1} ($x \approx 6$ Å), the corresponding values of the permittivity ε at a given pressure tend to the values of the dielectric constant given in the fourth column of table 1. On the other hand, these plots of ε reveal the state of dielectric saturation ($\varepsilon \to n^2$) achieved in high fields $E > 10^{10}$ V m^{-1} ($x < 1.5$ Å). Between these limiting values of the field (reduced distance) the permittivity ε at each pressure reveals an abrupt fall at $E \sim 10^9$ V m^{-1} ($x \sim 2.1$ Å). One can notice a similarity between the isobars $\varepsilon = \varepsilon(E)$ and $\varepsilon = \varepsilon(x)$ plotted in figures 1 and 2, respectively, for pressures p in the range $0.1 < p < 600$ MPa on the one hand and the isotherms $\varepsilon = \varepsilon(E)$ and $\varepsilon = \varepsilon(x)$ published in Ref. [5] (figures 3 and 4 therein, respectively) for temperatures in the range $273 < T < 373$ K on the other hand. However, the isobars and isotherms, although plotted against their corresponding abscissa in the same scale, differ in the degree in which they abruptly fall down at some place: the isobars fall down within a certain visible range of abscissa, whereas for isotherms the latter, within the applied scale, reduces to the line thickness.

   Note that in our calculations we have considered the nonlinear effects only due to the permanent moments of water molecules. A general discussion of nonlinear correction to induced dipole moments can be found in the literature (Ref. [6], p. 309).

Table 3. Permittivity ε of water for electric field strength E or reduced radius x under pressures 200, 300 and 400 MPa.

ε	$p = 200$ MPa		$p = 300$ MPa		$p = 400$ MPa	
	x (Å)	$10^{-9}E$ (V m^{-1})	x (Å)	$10^{-9}E$ (V m^{-1})	x (Å)	$10^{-9}E$ (V m^{-1})
2	0.620	187.089	0.559	229.924	0.498	289.697
2.5	1.106	47.065	1.063	50.927	1.024	54.852
3	1.334	26.919	1.294	28.635	1.258	30.294
4	1.574	14.503	1.534	15.268	1.500	15.983
5	1.702	9.925	1.662	10.409	1.628	10.855
6	1.782	7.544	1.742	7.896	1.708	8.218
7	1.838	6.084	1.797	6.361	1.763	6.612
10	1.933	3.849	1.892	4.017	1.857	4.168
15	2.004	2.388	1.963	2.489	1.928	2.579
20	2.039	1.730	1.997	1.802	1.962	1.867
25	2.061	1.355	2.019	1.411	1.984	1.462
30	2.078	1.110	2.036	1.156	2.001	1.198
35	2.097	0.934	2.053	0.974	2.017	1.010
40	2.119	0.801	2.074	0.836	2.036	0.867
45	2.148	0.693	2.100	0.725	2.060	0.753
50	2.185	0.603	2.133	0.632	2.091	0.658
55	2.234	0.524	2.176	0.552	2.130	0.576
60	2.299	0.453	2.233	0.480	2.181	0.504
65	2.389	0.388	2.310	0.415	2.250	0.437
70	2.516	0.325	2.417	0.352	2.342	0.374
73	–	–	2.503	0.315	–	–
75	2.713	0.261	–	–	2.475	0.313
76	–	–	2.614	0.277	–	–
79	–	–	2.767	0.238	–	–
80	3.071	0.191	–	–	2.681	0.250
81	–	–	2.907	0.210	–	–
83	–	–	3.100	0.180	–	–
84	3.774	0.120	–	–	–	–
85	–	–	3.394	0.147	3.068	0.180
86	5.003	0.067	–	–	–	–
86.4	5.750	0.050	–	–	–	–
86.9	11.543	0.012	–	–	–	–
87	–	–	3.947	0.106	–	–
88	–	–	–	–	3.582	0.127
89	–	–	6.428	0.039	–	–
89.3	–	–	12.224	0.011	–	–
91	–	–	–	–	6.410	0.038
91.3	–	–	–	–	13.633	0.008

4. Final remarks

The electric fields above 10^8 V m^{-1} can be encountered [3] in hydration layers arising when immersing in bulk water charged surfaces with surface charge density $\sigma_0 \geq 9 \times 10^{-4}$ C m^{-2}. Such charge densities can exist at the surface of flat or spherical (mercury droplets) metallic electrodes, oxides, at surfaces of proteins and micelles as well as at internal surfaces of reverse micelles. Such high local fields also exist around ions.

The knowledge of permittivity ε is needed to evaluate some thermodynamic quantities of hydration shells. The quantities in question comprise entropy, the related electrocaloric effect, as well as the local electrostriction and electrostriction pressure

Table 4.   Permittivity ε of water for electric field strength E or reduced radius x under pressures 500 and 600 MPa.

$p = 500$ MPa			$p = 600$ MPa		
ε	x (Å)	$10^{-9}E$ (V m^{-1})	ε	x (Å)	$10^{-9}E$ (V m^{-1})
2	0.435	379.124	2	0.370	524.162
2.5	0.989	58.782	2.5	0.959	62.606
3	1.227	31.861	3	1.200	33.291
4	1.470	16.629	4	1.446	17.191
5	1.599	11.251	5	1.575	11.588
6	1.679	8.501	6	1.656	8.739
7	1.734	6.831	7	1.711	7.015
10	1.829	4.299	10	1.807	4.406
15	1.900	2.657	15	1.877	2.720
20	1.934	1.922	20	1.912	1.967
25	1.955	1.505	25	1.933	1.539
30	1.972	1.233	30	1.949	1.262
35	1.988	1.040	35	1.965	1.065
40	2.006	0.894	40	1.982	0.915
45	2.028	0.777	45	2.003	0.797
50	2.056	0.680	50	2.029	0.699
55	2.093	0.597	55	2.063	0.614
60	2.140	0.523	60	2.106	0.540
65	2.201	0.456	65	2.163	0.473
70	2.284	0.394	70	2.237	0.410
75	2.400	0.333	71	2.255	0.398
80	2.573	0.272	74	2.316	0.362
83	2.728	0.233	78	2.421	0.315
86	2.961	0.191	80	2.488	0.290
89	3.377	0.142	82	2.569	0.266
92	4.673	0.072	85	2.728	0.227
93	8.764	0.020	90	3.226	0.154
			92.5	3.853	0.105
			93.5	4.426	0.079
			94.8	12.133	0.010

in hydration shells. Although, in experiments, temperature is a parameter much more frequently used than pressure, both of them play an equivalently important role as thermodynamic variables. Biochemical/biophysical experiments have shown [4] three possible pathways to protein denaturation by excessive heat, pressure, or coldness. The interest focused recently on various hydrated systems, as exemplified above, called for an approach that would lead to a description of the properties of hydration shells both in high electric fields and in sufficiently wide ranges of pressure. In this work, we have calculated the values of the permittivity $\varepsilon(E,p)$ in high fields in the range $10^8 < E < 10^{11}$ V m^{-1} of the electric field and in the range of pressures $0.1 < p < 600$ MPa included within the range of existence of the liquid phase of H_2O. No adjustable parameter was needed. The dielectric constant of pure water in the range of pressure investigated is known from the experiment. The results of this work can be helpful in proposing investigations of the effect of pressure on biosystems.

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Appendix

Table A1. Refractive index of water n as a function of the pressure p (MPa). Coefficients of fourth-order fitting polynomials in p to the data on Ref. [13], figure 3 therein: $n(p) = a_4 p^4 + a_3 p^3 + a_2 p^2 + a_1 p + a_0$.

a_0	a_1	a_2	a_3	a_4
+1.33310	$+1.10646 \times 10^{-4}$	-6.18547×10^{-8}	$+1.08380 \times 10^{-10}$	-8.17954×10^{-14}

Table A2. Specific volume of water v (m^3 kmol^{-1}) as a function of the pressure p (MPa). Coefficients of fourth-order fitting polynomials in p (MPa) to the data on Ref. [14]: $v(p) = a_4 p^4 + a_3 p^3 + a_2 p^2 + a_1 p + a_0$.

a_0	a_1	a_2	a_3	a_4
$+1.80466 \times 10^{-2}$	-7.89429×10^{-6}	$+4.63088 \times 10^{-9}$	$+1.65482 \times 10^{-12}$	-1.61981×10^{-15}

Table A3. Dielectric constant of water ε against pressure p. Coefficients of third-order fitting polynomials in p (MPa) at $T = 293$ K to the data from Ref. [15]: $\varepsilon(p) = a_3 p^3 + a_2 p^2 + a_1 p + a_0$.

a_0	a_1	a_2	a_3
+80.214	$+4.1866 \times 10^{-2}$	-4.7446×10^{-5}	$+3.0412 \times 10^{-8}$