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pH Determination Under Unconventional Conditions of Temperature and Ionic Strength

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Supplementary Information

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Appendix A

Nomenclature and use of equilibrium constants

Case 1. Non-leveled acid dissociation

Consider a non-leveled acid, HA, that partially dissociates according to the equilibrium presented in Eq. S1:

$$HA \rightleftarrows H^+ + A^- \qquad \text{Eq. S1}$$

HA represents a generic monoprotic acid dissociating into its Brønsted conjugate base, A^-, and hydronium ion, H_3O^+. For practical purposes, this species is denoted as H^+. Thus, the apparent acidity constant for this acid is written according to Eq. S2.

$$K_a = \frac{[H^+][A^-]}{[HA]} \qquad \text{Eq. S2}$$

By reversing the direction of the equilibrium reaction presented in Eq. S1, the equilibrium of Eq. S3, which corresponds to the formation of such acid.

$$A^- + H^+ \rightleftarrows HA \qquad \text{Eq. S3}$$

The nomenclature to designate the apparent global formation constant of the previous equilibrium is $\beta_{1,1}^{A^-|H^+}$. The superscripts indicate the polyreceptor and the exchanged particle, separated by the character pleca (|), in the context of the equilibrium of Eq. S3, the polyreceptor is A^-, and the exchanged particle is H^+. On the other hand, the subscripts indicate the reaction's stoichiometry, that is, the number of polyreceptors and particles necessary to form the product. The arrangement of these numbers corresponds to the position mentioned in the superscript. Thus, $1A^-$ and $1H^+$ are required to form HA. The apparent global formation constant of the HA acid (presented in Eq. S3), formed from the chemical entity A^- with exchanged H^+, is defined based on Eq. S4.

$$\beta_{1,1}^{A^-|H^+} = \frac{[HA]}{[A^-][H^+]} \qquad \text{Eq. S4}$$

This nomenclature has been used in other works, allowing the identification and manipulation of equilibrium constants in systems that involve polynuclear chemical entities and systems in the presence of condensed phases (Guerash-Briones et al. 2023).

The apparent global formation constant, $\beta_{1,1}^{A^-|H^+}$, is inversely proportional to the acidity constant, K_a (associated with the same equilibrium, but presented in opposite directions). The relationship between these constants is indicated in Eq. S5.

$$\beta_{1,1}^{A^-|H^+} = \frac{1}{K_a} \qquad \text{Eq. S5}$$

Finally, by applying logarithms on both sides, it is established that the logarithm of the apparent global formation constant, $\beta_{1,1}^{A^-|H^+}$, is equal to the pK_a of the acid–base pair HA/A^-; according to the first and last members of Eq. S6.

$$\log \beta_{1,1}^{A^-|H^+} = \log \frac{1}{K_a} = -\log K_a = pK_a \qquad \text{Eq. S6}$$

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Case 2. Dissociation of water

Autoprotolysis is called the chemical equilibrium in which water molecules are present to produce hydronium and hydroxide ions, according to the equilibrium presented in Eq. S7.

$$H_2O \rightleftarrows H^+ + OH^- \qquad \text{Eq. S7}$$

The autoionization constant is expressed as follows:

$$K_w = [H^+][OH^-] \qquad \text{Eq. S8}$$

The chemical equilibrium of Eq. S7 in the opposite direction will correspond to the global formation constant of water, $\beta_{1,1}^{OH^-|H^+}$, returning to the nomenclature presented previously. The expression of the law of mass action is expressed in Eq. S9.

$$\beta_{1,1}^{OH^-|H^+} = \frac{1}{[H^+][OH^-]} \qquad \text{Eq. S9}$$

The interdependence presented in Eq. S5 can be applied to the water system, where the overall formation constant of water formation, $\beta_{1,1}^{OH^-|H^+}$, is inversely proportional to the autoprotolysis constant Eq. S10.

$$\beta_{1,1}^{OH^-|H^+} = \frac{1}{K_w} \qquad \text{Eq. S10}$$

Consequently, we obtain Eq. S11 where the logarithm of the global formation constant of water is equal to the co-logarithm of the autoprotolysis constant, both at the same value of temperature and ionic strength.

$$\log \beta_{1,1}^{OH^-|H^+} = pK_w \qquad \text{Eq. S11}$$

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Appendix B

Table S1. Table of equivalence between salinity and ionic strength, expressed in mol L^{-1}, for selected temperature values.

Salinity [PSU]	**Temperature [°C]**													
	5.0	10.0	15.0	20.0	25.0	30.0	35.0	40.0	45.0	50.0	55.0	60.0	65.0	70.0
0.00005	0.000001	0.000001	0.000001	0.000001	0.000001	0.000001	0.000001	0.000001	0.000001	0.000001	0.000001	0.000001	0.000001	0.000001
0.0005	0.000010	0.000010	0.000010	0.000010	0.000010	0.000010	0.000010	0.000010	0.000010	0.000010	0.000010	0.000010	0.000010	0.000010
0.005	0.000103	0.000103	0.000103	0.000103	0.000103	0.000103	0.000103	0.000102	0.000102	0.000102	0.000102	0.000102	0.000101	0.000101
0.05	0.001032	0.001032	0.001031	0.001031	0.001029	0.001028	0.001026	0.001024	0.001022	0.001020	0.001018	0.001015	0.001013	0.001010
0.5	0.010327	0.010324	0.010318	0.010309	0.010297	0.010282	0.010266	0.010247	0.010226	0.010204	0.010180	0.010155	0.010130	0.010105
1.0	0.020662	0.020657	0.020644	0.020625	0.020601	0.020572	0.020539	0.020501	0.020460	0.020415	0.020368	0.020319	0.020268	0.020218
2.5	0.051718	0.051702	0.051669	0.051622	0.051561	0.051488	0.051404	0.051310	0.051207	0.051095	0.050977	0.050854	0.050728	0.050602
5.0	0.103640	0.103605	0.103537	0.103440	0.103316	0.103168	0.102999	0.102810	0.102602	0.102379	0.102142	0.101896	0.101646	0.101396
7.5	0.155767	0.155709	0.155603	0.155453	0.155264	0.155040	0.154784	0.154499	0.154187	0.153851	0.153496	0.153128	0.152753	0.152381
10.0	0.208097	0.208014	0.207865	0.207661	0.207405	0.207104	0.206760	0.206377	0.205959	0.205511	0.205038	0.204547	0.204049	0.203556
12.0	0.250109	0.250001	0.249818	0.249568	0.249258	0.248893	0.248477	0.248016	0.247513	0.246974	0.246406	0.245818	0.245221	0.244632
14.5	0.302806	0.302666	0.302437	0.302128	0.301747	0.301301	0.300796	0.300235	0.299625	0.298972	0.298285	0.297575	0.296856	0.296148
17.5	0.366311	0.366129	0.365840	0.365457	0.364990	0.364445	0.363829	0.363148	0.362409	0.361619	0.360788	0.359932	0.359067	0.358216
20.0	0.419457	0.419235	0.418894	0.418447	0.417906	0.417277	0.416568	0.415785	0.414936	0.414031	0.413081	0.412102	0.411115	0.410148
25.0	0.526361	0.526050	0.525597	0.525016	0.524320	0.523518	0.522619	0.521630	0.520560	0.519422	0.518231	0.517007	0.515778	0.514578
30.0	0.634083	0.633672	0.633097	0.632373	0.631516	0.630535	0.629439	0.628238	0.626944	0.625570	0.624135	0.622666	0.621195	0.619764
34.0	0.720851	0.720352	0.719672	0.718828	0.717836	0.716707	0.715451	0.714078	0.712600	0.711035	0.709404	0.707737	0.706073	0.704459
35.0	0.742626	0.742103	0.741396	0.740521	0.739495	0.738329	0.737032	0.735615	0.734091	0.732478	0.730798	0.729081	0.727368	0.725709
40.0	0.851993	0.851347	0.850498	0.849464	0.848263	0.846905	0.845401	0.843763	0.842006	0.840150	0.838221	0.836255	0.834299	0.832413
45.0	0.962188	0.961408	0.960407	0.959207	0.957823	0.956267	0.954551	0.952687	0.950692	0.948589	0.946408	0.944191	0.941992	0.939880
50.0	1.073214	1.072288	1.071127	1.069752	1.068179	1.066419	1.064485	1.062391	1.060154	1.057800	1.055364	1.052893	1.050449	1.048111
55.0	1.185075	1.183992	1.182663	1.181105	1.179336	1.177367	1.175210	1.172879	1.170395	1.167786	1.165091	1.162363	1.159673	1.157109
60.0	1.297774	1.296525	1.295018	1.293271	1.291300	1.289115	1.286729	1.284157	1.281421	1.278552	1.275594	1.272607	1.269668	1.266877
65.0	1.411316	1.409891	1.408197	1.406254	1.404073	1.401667	1.399047	1.396228	1.393235	1.390102	1.386877	1.383627	1.380437	1.377419
70.0	1.525706	1.524095	1.522206	1.520058	1.517662	1.515029	1.512168	1.509098	1.505843	1.502441	1.498945	1.495428	1.491985	1.488738

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In Fig. S1, the response surface is shown, establishing the relationship between salinity and ionic strength values in the defined temperature range. It is observed that the surface exhibits a slight curvature at extremely high and low salinity and ionic strength ranges, indicating that salinity and ionic strength do not vary proportionally under these conditions.

https://qr4.at/rMzMHc

Fig. S1. QR code for the response surface for the equivalence between salinity and ionic strength values for the proposed temperature range.

Appendix C

Determination of pH through the solution of a third−degree polynomial

This polynomial allows the determination of $[H^+]$ in a solution prepared either from the acid, an alkaline metal salt of the conjugate base, or both. Its derivation is described in the following steps.

First, the apparent acidity constant of the conjugate pair HA/A^- associated with the equilibrium $HA \rightleftarrows H^+ + A^-$, where HA represents a generic acidic species, and A^- represents its respective conjugate base, is considered (Eq. S12).

$$K_a = \frac{1}{\beta_{1,1}^{A^-|H^+}} = \frac{[H^+][A^-]}{[HA]} \qquad \text{Eq. S12}$$

Next, the apparent constant for water formation, $H^+ + OH^- \rightleftarrows H_2O$ (Eq. S13), where K_w is the apparent constant for the autoprotolysis of water, is considered. For simplicity, this work prefers the notation $[H^+]$ instead of $[H_3O^+]$ to denote the effective molar concentration of hydronium ions. This equilibrium is obtained by removing one water molecule from each side of the equality defining K_w.

$$\beta_{1,1}^{OH^-|H^+} = \frac{1}{[H^+][OH^-]} = \frac{1}{K_w} \qquad \text{Eq. S13}$$

Note that the origin of the conjugate base may also be due to the presence of a strong electrolyte, such as a potassium salt. In such a case, Eq. S14 can be established based on the equilibrium of solution formation, $KA \longrightarrow K^+ + A^-$.

$$C_{KA} = [K^+] \qquad \text{Eq. S14}$$

In the case of a solution where both the acid and the conjugate base are present, equilibrium Eq. S15, can be established, which is valid regardless of the origin of the acidic species and the alkaline species.

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$$C_{\text{buffer}} = [HA] + [A^-] \qquad \text{Eq. S15}$$

The charge balance (or, according to some texts, the principle of electroneutrality on a solution) postulates that a solution is electrically neutral. Mathematically, it is shown by an expression where the sum of the effective molar concentrations of the cations, each one multiplied by the absolute value of their charge, is equal to the sum of the effective molar concentrations of the anions, each one multiplied by the absolute value of its charge (Castellan, 1983; Burgot, 2012; Butler, 1998). Thus, the charge balance is fulfilled regardless of the origin of the chemical species. This relationship is represented in Eq. S16, where the *i*–th cationic species and the *j*–th anionic species are represented.

$$\sum |z_i|[i^{z+}] = \sum |z_j|[j^{z-}] \qquad \text{Eq. S16}$$

Thus, Eq. S17 presents the charge balance of a solution of a potassium salt of a conjugate base (KA) that exhibits the behavior of a true electrolyte, accompanied by the acidic particle and the basic particle of the water. In the presence of any true univalent electrolyte used to fix ionic strength, and whose constituent ions are chemically inert, these ions will appear on both sides of the equation, resulting in no net contribution to the charge balance.

$$[A^-] + [OH^-] = [H^+] + [K^+] \qquad \text{Eq. S17}$$

First, the effective molar concentration of the conjugate base, $[A^-]$, is determined from Eq. S17 and the molar concentration of the alkaline metal, $[K^+]$, is replaced with the analytical concentration of Eq. S14.

$$[A^-] = C_{KA} + [H^+] - [OH^-] \qquad \text{Eq. S18}$$

On the other hand, [HA] is determined from Eq. S15 and the term $[A^-]$ is replaced with the calculation presented in Eq. S18.

$$\begin{gathered}[HA] = C_{\text{buffer}} - [A^-] \\ [HA] = (C_{HA} + C_{KA}) - (C_{KA} + [H^+] - [OH^-])\end{gathered} \qquad \text{Eq. S19}$$

This results in Eq. S20.

$$[HA] = C_{HA} - [H^+] + [OH^-] \qquad \text{Eq. S20}$$

Then, the expression for the law of mass action of the acidity constant for the conjugate pair HA/A^- (Eq. S12) is taken, and $[H^+]$ is determined.

$$[H^+] = K_a \frac{[HA]}{[A^-]} \qquad \text{Eq. S21}$$

The numerator (Eq. S20) and the denominator (Eq. S18) are identifiable, and they are then substituted into Eq. S21.

$$[H^+] = K_a \frac{(C_{HA} - [H^+] + [OH^-])}{(C_{KA} + [H^+] - [OH^-])} \qquad \text{Eq. S22}$$

The $[OH^-]$ is determined from Eq. S13 to express Eq. S22 solely in terms of $[H^+]$, the initial

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concentration of the acid, C_{HA}, the initial concentration of the base, C_{KA}, and the apparent acidity constant.

$$[H^+] = K_a \frac{\left(C_{HA} - [H^+] + \frac{K_w}{[H^+]}\right)}{\left([H^+] - \frac{K_w}{[H^+]}\right)} \quad \text{Eq. S23}$$

From Eq. S23 two cases arise. The first, when the solution is prepared solely from the acid, $C_{HA} = C_0$, and consequently, $C_{KA} = 0$ mol L^{-1}, resulting in Eq. S24.

$$[H^+] = K_a \frac{\left(C_{HA} - [H^+] + \frac{K_w}{[H^+]}\right)}{\left([H^+] - \frac{K_w}{[H^+]}\right)} \quad \text{Eq. S24}$$

The linear version of the above expression is a third−degree polynomial (Eq. S25) whose positive root satisfying the condition $[H^+] \in \mathbb{R}^+$ is linked to the pH value.

$$[H^+]^3 + K_a[H^+]^2 + (-K_w - K_a C_0)[H^+] - K_a K_w = 0 \quad \text{Eq. S25}$$

The second case arises when the solution is prepared solely from a salt of an alkaline metal of the conjugate base, $C_{KA} = C_0$, and consequently, $C_{HA} = 0$ mol L^{-1}. Eq. S26 is obtained.

$$[H^+] = K_a \frac{\left(-[H^+] + \frac{K_w}{[H^+]}\right)}{\left(C_{KA} + [H^+] - \frac{K_w}{[H^+]}\right)} \quad \text{Eq. S26}$$

The linear version of the above expression is the other third−degree polynomial (Eq. S27) whose positive root satisfying the condition $[H^+] \in \mathbb{R}^+$ is again linked to the pH value.

$$[H^+]^3 + (K_a + C_0)[H^+]^2 - K_w[H^+] - K_a K_w = 0 \quad \text{Eq. S27}$$

In either case, Eq. S28 is satisfied, making the value of the logarithm of the apparent formation constant applicable, in terms of K_a, in the above expressions.

$$\log\left(\beta_{1,1}^{A^-|H^+}\Big|_{I>0}\right) = pK_a(H^+/A^-)|_{I>0} \quad \text{Eq. S28}$$

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Appendix D

Relative percentage differences calculated for $\Delta_r H°$ and $\Delta_r S°$

Table S2. Comparison of the thermodynamic parameters for the equilibrium $H^+ + OH^- \rightleftarrows H_2O$ obtained by the proposed non−linear fit in this work and the reported values. The relative difference (%) is added only as a plain comparison criterion.

	$\Delta_r H°$ (J mol^{-1})	**$\Delta_r S°$ (J mol^{-1} K^{-1})**	**$\Delta C_p°$ (J mol^{-1} K^{-1})**	**Coefficient of determination**	**Linear range**
Non−linear function	− 57 563.93	74.77	264.17	0.99987	0.0 ≤ T [°C] ≤ 100
Reported values (Martell & Smith, 1982)	− 55 814.56	80.75		N/A	0.0 ≤ T [°C] ≤ 60
Relative difference (%)	3.13	7.41		N/A	N/A

Table S3. Comparison of the thermodynamic parameters for the equilibrium $CH_3COO^- + H^+ \rightleftarrows CH_3COOH$ obtained by the proposed non−linear fit in this work and the reported values. The relative difference (%) is added only as a plain comparison criterion.

	$\Delta_r H°$ (J mol^{-1})	**$\Delta_r S°$ (J mol^{-1} K^{-1})**	**$\Delta C_p°$ (J mol^{-1} K^{-1})**	**Coefficient of determination**	**Linear range**
Non−linear function	440.48	92.52	155.25	0.99934	0.0 ≤ T [°C] ≤ 60
Reported values (Martell & Smith, 1982)	418.40	92.47		N/A	0.0 ≤ T [°C] ≤ 60
Relative difference (%)	5.28	0.05		N/A	N/A

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Appendix E

Table S4. Table of values of the logarithm of the apparent autoprotolysis constant of water (pK_w) for selected temperature and salinity values.

Salinity	**Temperature [°C]**													
[PSU]	5.0	10.0	15.0	20.0	25.0	30.0	35.0	40.0	45.0	50.0	55.0	60.0	65.0	70.0
0.0	14.7492	14.5430	14.3481	14.1640	13.9900	13.8256	13.6702	13.5233	13.3845	13.2534	13.1295	13.0125	12.9020	12.7977
0.00005	14.7482	14.5420	14.3471	14.1630	13.9890	13.8246	13.6691	13.5223	13.3835	13.2523	13.1284	13.0114	12.9009	12.7966
0.005	14.7393	14.5329	14.3380	14.1538	13.9797	13.8152	13.6597	13.5128	13.3739	13.2426	13.1186	13.0015	12.8909	12.7865
0.5	14.6534	14.4464	14.2508	14.0659	13.8911	13.7258	13.5695	13.4217	13.2820	13.1499	13.0251	12.9070	12.7955	12.6901
1.0	14.6161	14.4088	14.2129	14.0276	13.8525	13.6869	13.5303	13.3822	13.2421	13.1096	12.9844	12.8660	12.7540	12.6482
2.0	14.5654	14.3577	14.1614	13.9757	13.8002	13.6341	13.4771	13.3285	13.1879	13.0550	12.9292	12.8103	12.6978	12.5914
4.0	14.4975	14.2893	14.0925	13.9063	13.7302	13.5636	13.4059	13.2567	13.1155	12.9819	12.8555	12.7358	12.6226	12.5155
6.0	14.4482	14.2397	14.0425	13.8559	13.6794	13.5124	13.3543	13.2046	13.0630	12.9289	12.8020	12.6818	12.5681	12.4604
8.0	14.4084	14.1996	14.0020	13.8152	13.6383	13.4710	13.3126	13.1626	13.0206	12.8861	12.7588	12.6382	12.5241	12.4159
10.0	14.3745	14.1654	13.9676	13.7805	13.6034	13.4358	13.2771	13.1268	12.9845	12.8497	12.7221	12.6012	12.4866	12.3781
15.0	14.3057	14.0962	13.8979	13.7103	13.5327	13.3645	13.2052	13.0543	12.9114	12.7760	12.6477	12.5261	12.4108	12.3016
20.0	14.2510	14.0411	13.8425	13.6544	13.4764	13.3078	13.1481	12.9967	12.8533	12.7174	12.5886	12.4665	12.3506	12.2408
25.0	14.2050	13.9948	13.7959	13.6076	13.4292	13.2602	13.1001	12.9484	12.8046	12.6683	12.5390	12.4164	12.3001	12.1898
30.0	14.1651	13.9546	13.7555	13.5669	13.3882	13.2189	13.0585	12.9065	12.7623	12.6256	12.4960	12.3730	12.2563	12.1455
35.0	14.1296	13.9190	13.7196	13.5307	13.3518	13.1823	13.0216	12.8693	12.7248	12.5878	12.4579	12.3345	12.2175	12.1063
40.0	14.0976	13.8868	13.6872	13.4981	13.3190	13.1493	12.9883	12.8357	12.6910	12.5537	12.4235	12.2999	12.1825	12.0710
45.0	14.0684	13.8574	13.6577	13.4684	13.2891	13.1191	12.9580	12.8051	12.6602	12.5226	12.3921	12.2682	12.1505	12.0387
50.0	14.0415	13.8304	13.6304	13.4410	13.2615	13.0913	12.9300	12.7769	12.6318	12.4940	12.3632	12.2391	12.1211	12.0090
55.0	14.0164	13.8052	13.6051	13.4156	13.2359	13.0655	12.9040	12.7508	12.6054	12.4674	12.3364	12.2120	12.0938	11.9815
60.0	13.9931	13.7817	13.5815	13.3918	13.2120	13.0414	12.8797	12.7263	12.5808	12.4426	12.3114	12.1868	12.0684	11.9558
65.0	13.9711	13.7596	13.5593	13.3694	13.1895	13.0188	12.8569	12.7034	12.5576	12.4193	12.2879	12.1631	12.0444	11.9316
70.0	13.9503	13.7388	13.5383	13.3483	13.1682	12.9974	12.8354	12.6817	12.5358	12.3973	12.2657	12.1407	12.0218	11.9088

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Appendix F

Table S5. Tabulated values of the logarithm of the apparent dissociation constant of acetic acid ($pK_a(CH_3COOH/CH_3COO^-)$) for selected temperature and salinity values.

Salinity [PSU]	**Temperature [°C]**													
	5.0	10.0	15.0	20.0	25.0	30.0	35.0	40.0	45.0	50.0	55.0	60.0	65.0	70.0
0.0	4.7701	4.7625	4.7577	4.7554	4.7556	4.7580	4.7625	4.7689	4.7772	4.7872	4.7988	4.8119	4.8264	4.8422
0.00005	4.7691	4.7615	4.7567	4.7544	4.7546	4.7569	4.7614	4.7678	4.7761	4.7861	4.7977	4.8108	4.8253	4.8411
0.005	4.7601	4.7525	4.7476	4.7452	4.7453	4.7476	4.7520	4.7583	4.7665	4.7764	4.7879	4.8009	4.8153	4.8310
0.5	4.6747	4.6664	4.6608	4.6577	4.6571	4.6586	4.6622	4.6678	4.6751	4.6842	4.6948	4.7069	4.7203	4.7351
1.0	4.6378	4.6292	4.6233	4.6199	4.6189	4.6202	4.6234	4.6286	4.6356	4.6443	4.6546	4.6663	4.6793	4.6937
2.0	4.5878	4.5788	4.5726	4.5688	4.5674	4.5682	4.5710	4.5758	4.5823	4.5905	4.6002	4.6114	4.6240	4.6377
4.0	4.5213	4.5119	4.5051	4.5008	4.4989	4.4991	4.5013	4.5055	4.5114	4.5190	4.5280	4.5385	4.5504	4.5634
6.0	4.4733	4.4635	4.4563	4.4517	4.4494	4.4492	4.4510	4.4548	4.4602	4.4673	4.4759	4.4860	4.4973	4.5098
8.0	4.4347	4.4245	4.4171	4.4122	4.4095	4.4091	4.4106	4.4140	4.4191	4.4258	4.4340	4.4437	4.4546	4.4666
10.0	4.4019	4.3915	4.3839	4.3787	4.3758	4.3750	4.3763	4.3794	4.3842	4.3906	4.3985	4.4078	4.4184	4.4301
15.0	4.3357	4.3249	4.3168	4.3111	4.3077	4.3064	4.3071	4.3096	4.3139	4.3197	4.3270	4.3356	4.3455	4.3565
20.0	4.2833	4.2722	4.2637	4.2577	4.2539	4.2522	4.2525	4.2546	4.2583	4.2637	4.2705	4.2786	4.2879	4.2983
25.0	4.2395	4.2281	4.2193	4.2130	4.2089	4.2069	4.2068	4.2085	4.2119	4.2169	4.2233	4.2310	4.2398	4.2498
30.0	4.2016	4.1900	4.1810	4.1744	4.1700	4.1677	4.1673	4.1688	4.1718	4.1765	4.1825	4.1898	4.1983	4.2079
35.0	4.1680	4.1563	4.1470	4.1402	4.1356	4.1331	4.1324	4.1336	4.1364	4.1407	4.1464	4.1534	4.1616	4.1708
40.0	4.1379	4.1259	4.1165	4.1095	4.1047	4.1019	4.1011	4.1020	4.1045	4.1086	4.1140	4.1207	4.1286	4.1375
45.0	4.1104	4.0983	4.0887	4.0815	4.0766	4.0736	4.0725	4.0732	4.0756	4.0794	4.0846	4.0910	4.0986	4.1072
50.0	4.0851	4.0729	4.0632	4.0558	4.0507	4.0476	4.0463	4.0468	4.0489	4.0525	4.0575	4.0637	4.0711	4.0794
55.0	4.0617	4.0494	4.0395	4.0320	4.0267	4.0234	4.0220	4.0223	4.0243	4.0277	4.0324	4.0384	4.0455	4.0536
60.0	4.0399	4.0274	4.0175	4.0098	4.0044	4.0009	3.9994	3.9995	4.0013	4.0045	4.0091	4.0149	4.0218	4.0296
65.0	4.0194	4.0068	3.9968	3.9890	3.9834	3.9798	3.9781	3.9781	3.9797	3.9828	3.9872	3.9928	3.9995	4.0071
70.0	4.0001	3.9874	3.9773	3.9694	3.9637	3.9600	3.9581	3.9580	3.9594	3.9623	3.9665	3.9720	3.9785	3.9859

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Appendix G

Table S6. Tabulated pH values for an acetic acid solution prepared at an analytical concentration of $C_0 = 0.1$ mol L^{-1} for selected temperature and salinity values.

Salinity	**Temperature [°C]**													
[PSU]	5.0	10.0	15.0	20.0	25.0	30.0	35.0	40.0	45.0	50.0	55.0	60.0	65.0	70.0
0	2.888	2.884	2.882	2.881	2.881	2.882	2.884	2.887	2.891	2.896	2.902	2.909	2.916	2.924
0.00005	2.887	2.884	2.881	2.880	2.880	2.881	2.884	2.887	2.891	2.896	2.902	2.908	2.915	2.923
0.005	2.883	2.879	2.877	2.876	2.876	2.877	2.879	2.882	2.886	2.891	2.897	2.903	2.910	2.918
0.5	2.841	2.836	2.834	2.832	2.832	2.833	2.834	2.837	2.841	2.845	2.850	2.856	2.863	2.870
1.0	2.822	2.818	2.815	2.813	2.813	2.813	2.815	2.818	2.821	2.825	2.831	2.836	2.843	2.850
2.0	2.797	2.793	2.790	2.788	2.787	2.788	2.789	2.791	2.795	2.799	2.804	2.809	2.815	2.822
4.0	2.764	2.760	2.756	2.754	2.753	2.753	2.755	2.757	2.760	2.763	2.768	2.773	2.779	2.785
6.0	2.741	2.736	2.732	2.730	2.729	2.729	2.730	2.731	2.734	2.738	2.742	2.747	2.753	2.759
8.0	2.721	2.716	2.713	2.710	2.709	2.709	2.710	2.711	2.714	2.717	2.721	2.726	2.731	2.737
10.0	2.705	2.700	2.696	2.694	2.692	2.692	2.693	2.694	2.697	2.700	2.704	2.708	2.713	2.719
15.0	2.672	2.667	2.663	2.660	2.659	2.658	2.658	2.660	2.662	2.665	2.668	2.672	2.677	2.683
20.0	2.647	2.641	2.637	2.634	2.632	2.631	2.631	2.632	2.634	2.637	2.640	2.644	2.649	2.654
25.0	2.625	2.619	2.615	2.612	2.610	2.609	2.609	2.610	2.611	2.614	2.617	2.621	2.625	2.630
30.0	2.606	2.601	2.596	2.593	2.591	2.590	2.589	2.590	2.592	2.594	2.597	2.600	2.605	2.609
35.0	2.590	2.584	2.579	2.576	2.574	2.572	2.572	2.573	2.574	2.576	2.579	2.582	2.586	2.591
40.0	2.575	2.569	2.564	2.561	2.558	2.557	2.557	2.557	2.558	2.560	2.563	2.566	2.570	2.575
45.0	2.561	2.555	2.551	2.547	2.545	2.543	2.543	2.543	2.544	2.546	2.549	2.552	2.555	2.560
50.0	2.549	2.543	2.538	2.534	2.532	2.530	2.530	2.530	2.531	2.533	2.535	2.538	2.542	2.546
55.0	2.537	2.531	2.526	2.523	2.520	2.518	2.518	2.518	2.519	2.520	2.523	2.526	2.529	2.533
60.0	2.527	2.520	2.515	2.512	2.509	2.507	2.507	2.507	2.507	2.509	2.511	2.514	2.518	2.521
65.0	2.516	2.510	2.505	2.501	2.499	2.497	2.496	2.496	2.497	2.498	2.501	2.503	2.507	2.510
70.0	2.507	2.501	2.496	2.492	2.489	2.487	2.486	2.486	2.487	2.488	2.490	2.493	2.496	2.500

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Appendix H

Table S7. Tabulated pH values for a potassium acetate solution prepared at an analytical concentration of $C_0 = 0.1$ mol L^{-1} for selected temperature and salinity values.

Salinity	**Temperature [°C]**													
[PSU]	5.0	10.0	15.0	20.0	25.0	30.0	35.0	40.0	45.0	50.0	55.0	60.0	65.0	70.0
0	9.260	9.153	9.053	8.960	8.873	8.792	8.716	8.646	8.581	8.520	8.464	8.412	8.364	8.320
0.00005	9.259	9.152	9.052	8.959	8.872	8.791	8.715	8.645	8.580	8.519	8.463	8.411	8.363	8.319
0.005	9.250	9.143	9.043	8.950	8.863	8.781	8.706	8.636	8.570	8.510	8.453	8.401	8.353	8.309
0.5	9.164	9.056	8.956	8.862	8.774	8.692	8.616	8.545	8.479	8.417	8.360	8.307	8.258	8.213
1.0	9.127	9.019	8.918	8.824	8.736	8.654	8.577	8.505	8.439	8.377	8.319	8.266	8.217	8.171
2.0	9.077	8.968	8.867	8.772	8.684	8.601	8.524	8.452	8.385	8.323	8.265	8.211	8.161	8.115
4.0	9.009	8.901	8.799	8.704	8.615	8.531	8.454	8.381	8.314	8.250	8.192	8.137	8.086	8.039
6.0	8.961	8.852	8.749	8.654	8.564	8.481	8.403	8.330	8.262	8.198	8.139	8.084	8.033	7.985
8.0	8.922	8.812	8.710	8.614	8.524	8.440	8.362	8.288	8.220	8.156	8.096	8.041	7.989	7.941
10.0	8.888	8.779	8.676	8.580	8.490	8.405	8.327	8.253	8.184	8.120	8.060	8.005	7.953	7.904
15.0	8.821	8.711	8.607	8.511	8.420	8.336	8.256	8.182	8.113	8.048	7.987	7.931	7.878	7.829
20.0	8.767	8.657	8.553	8.456	8.365	8.280	8.200	8.126	8.056	7.991	7.930	7.873	7.819	7.770
25.0	8.722	8.612	8.508	8.410	8.319	8.234	8.154	8.079	8.008	7.943	7.881	7.824	7.770	7.720
30.0	8.683	8.572	8.468	8.371	8.279	8.193	8.113	8.038	7.967	7.901	7.839	7.781	7.727	7.677
35.0	8.649	8.538	8.433	8.336	8.244	8.158	8.077	8.002	7.931	7.864	7.802	7.744	7.690	7.639
40.0	8.618	8.507	8.402	8.304	8.212	8.126	8.045	7.969	7.898	7.831	7.769	7.710	7.656	7.604
45.0	8.590	8.478	8.373	8.275	8.183	8.097	8.015	7.939	7.868	7.801	7.738	7.680	7.625	7.573
50.0	8.563	8.452	8.347	8.249	8.156	8.070	7.988	7.912	7.841	7.773	7.711	7.652	7.596	7.544
55.0	8.539	8.427	8.323	8.224	8.131	8.045	7.963	7.887	7.815	7.748	7.685	7.625	7.570	7.518
60.0	8.517	8.405	8.300	8.201	8.108	8.021	7.940	7.863	7.791	7.724	7.660	7.601	7.545	7.493
65.0	8.495	8.383	8.278	8.179	8.087	8.000	7.918	7.841	7.769	7.701	7.638	7.578	7.522	7.470
70.0	8.475	8.363	8.258	8.159	8.066	7.979	7.897	7.820	7.748	7.680	7.616	7.556	7.500	7.448

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Appendix I

Comparison between response surfaces

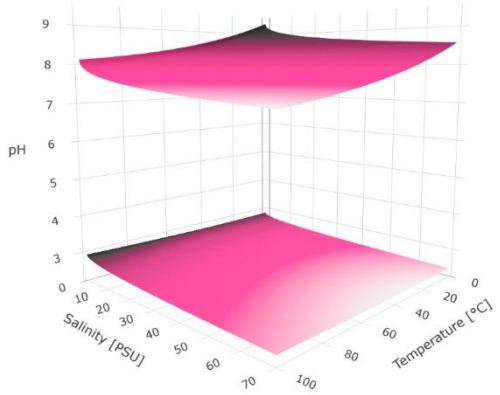

Fig. S2. Response surfaces of pH for an acetic acid solution (bottom) and a potassium acetate solution (top), both at $C_0 = 0.1$ mol L^{-1}, for the proposed temperature ($5.0 \leq T[°C] \leq 100.0$) and salinity ($0.0 \leq Sp[PSU] \leq 70.0$) intervals.

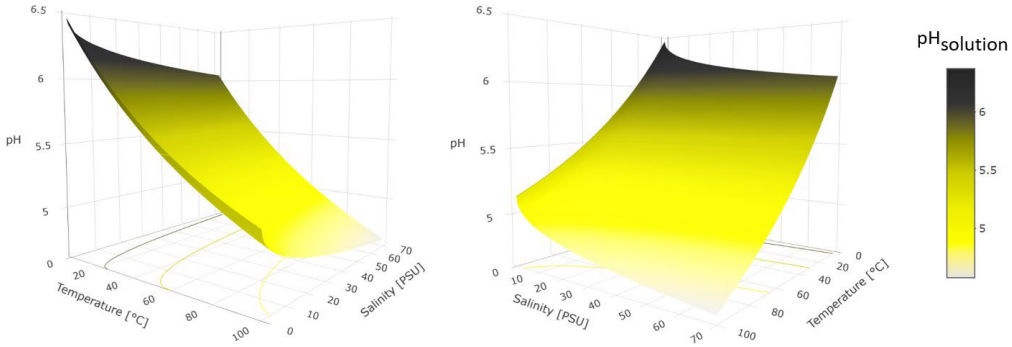

Fig. S3. Two perspectives of the response surfaces for the pH difference between acetic acid and potassium acetate solutions, both at $C_0 = 0.1$ mol L^{-1}, for the proposed temperature ($5.0 \leq T[°C] \leq 100.0$) and salinity ($0.0 \leq Sp[PSU] \leq 70.0$) intervals.

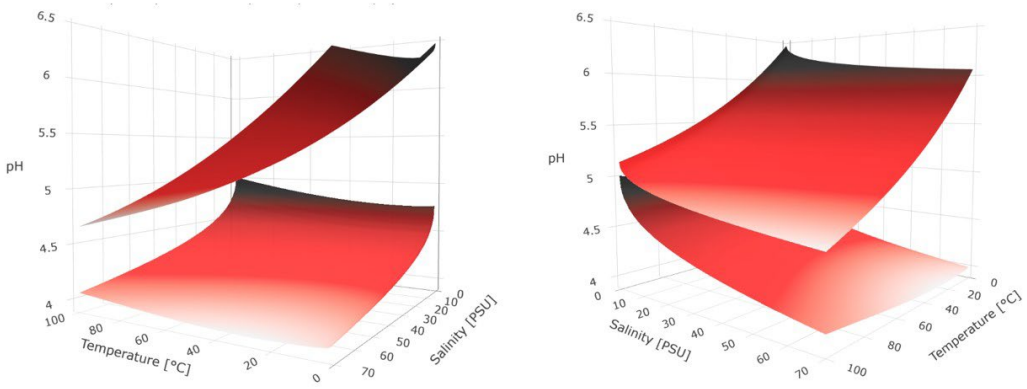

Fig. S4. Two perspectives of the comparison of the response surface for the pH difference between acetic acid

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and potassium acetate solutions (top), both at $C_0 = 0.1$ mol L^{-1}, and the response surface of the logarithm of the apparent formation constant for the $CH_3COO^- + H^+ \rightleftarrows CH_3COOH$ equilibrium (bottom), for the proposed temperature ($5.0 \leq T[°C] \leq 110.0$) and salinity ($0.0 \leq Sp[PSU] \leq 70.0$) intervals.

Appendix J

Interactive 3D surfaces. To efficiently view the 3D graphics created in RStudio, it is recommended to scan the QR code, download the HTML file, and finally open it with a proper web browser.

https://qr4.at/jgofzV

Fig. S5. QR code for the response surface of the logarithm of the apparent formation constant for the $H^+ + OH^- \rightleftarrows H_2O$ equilibrium within the proposed temperature intervals ($5.0 \leq T[°C] \leq 100.0$) and salinity ($0.0 \leq Sp[PSU] \leq 70.0$).

https://qr4.at/JRc6eT

Fig. S6. QR code for the response surface of the logarithm of the apparent formation constant for the $CH_3COO^- + H^+ \rightleftarrows CH_3COOH$ equilibrium within the proposed temperature intervals ($0.0 \leq T[°C] \leq 60.0$) and salinity ($0.0 \leq Sp[PSU] \leq 70.0$).

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https://qr4.at/FIiNJW

Fig. S7. QR code for the response surface of the pH of an acetic acid solution, C_0 = 0.1 mol L^{-1}, within the proposed temperature intervals (5.0 ≤ T[°C] ≤ 100.0) and salinity (0.0 ≤ Sp[PSU] ≤ 70.0).

https://qr4.at/jI2x0A

Fig. S8. QR code for the response surface of the pH of a potassium acetate solution, C_0 = 0.1 mol L^{-1}, within the proposed temperature intervals (5.0 ≤ T[°C] ≤ 100.0) and salinity (0.0 ≤ Sp[PSU] ≤ 70.0).

https://qr4.at/xUFHZS

Fig. S9. QR code for the response surfaces of pH for an acetic acid solution (bottom) and a potassium acetate solution (top), both at C_0 = 0.1 mol L^{-1}, within the proposed temperature intervals (5.0 ≤ T[°C] ≤ 100.0) and salinity (0.0 ≤ Sp[PSU] ≤ 70.0).

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https://qr4.at/h79VnS

Fig. S10. QR code for the response surfaces for the pH difference between acetic acid and potassium acetate solutions, both at C_0 = 0.1 mol L^{-1}, for the proposed temperature (5.0 ≤ T[°C] ≤ 100.0) and salinity (0.0 ≤ Sp[PSU] ≤ 70.0) intervals.

https://qr4.at/8eWuvK

Fig. S11. QR code for the comparison of the response surface for the pH difference between acetic acid and potassium acetate solutions (top), both at C_0 = 0.1 mol L^{-1}, and the response surface of the logarithm of the apparent formation constant for the $CH_3COO^- + H^+ \rightleftarrows CH_3COOH$ equilibrium (bottom), for the proposed temperature (5.0 ≤ T[°C] ≤ 110.0) and salinity (0.0 ≤ Sp[PSU] ≤ 70.0) intervals.