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*Research Article*

# Volumetric Properties for the Aqueous Solution of Yttrium Trichloride at Temperatures from 283.15 to 363.15 K and Ambient Pressure

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To effectively develop the rare earth elements resources from the geothermal waters, it is essential to understand the volumetric properties of the aqueous solution system to establish the relative thermodynamic model. In this study, densities of $YCl_3$ (aq) at the molalities of 0.08837–1.60639 mol·kg$^{-1}$ from 283.15 K to 363.15 K at 5 K intervals and ambient pressure were measured experimentally by an Anton Paar digital vibrating-tube densimeter. Based on experimental data, the volumetric properties including apparent molar volume ($V_\phi$) and the coefficient of thermal expansion of the solution ($\alpha$) of the binary systems ($YCl_3 + H_2O$) were derived. The 3D diagram ($m_i$, $T$, $V_\phi$) of apparent molar volumes against temperature and molality was plotted. On the basis of the Pitzer ion-interaction model of electrolyte, the Pitzer single-salt parameters ($\beta^{(0)v}_{MX}$, $\beta^{(1)v}_{MX}$, and $C^v_{MX}$) for $YCl_3$ and temperature-dependence equation $F(i,\ p,\ T) = a_1 + a_2\ln(T/298.15) + a_3(T\text{-}298.15) + a_4/(620\text{-}T) + a_5(T\text{-}227)$ as well as their coefficients $a_i$ ($i$ = 1–5) in the binary system were obtained for the first time. The values of Pitzer single-salt parameters of $YCl_3$ agree well with the calculated values corresponding to the temperature-dependence equations, indicating that single-salt parameters and temperature-dependent formula obtained in this work are reliable.

## 1. Introduction

Rare earth elements (REEs) are vital ingredients of modern technologies, especially in energy, environmental protection, digital technology, the nuclear industry, and medical applications. REEs are also an integral part of electronic devices serving as magnets, catalysts, and superconductors, owing to their chemical, catalytic, electrical, magnetic, and optical properties [1–7]. What is more, in nuclear medicine, many radioisotopes such as yttrium have been used in diagnostic or therapeutic procedures to treat a wide range of diseases, including cancer [8]. The continuously increasing demand for yttrium has led to the high economic importance of yttrium. Tibet is one of the famous geothermally active regions, and the geothermal water resources with high concentrations of rare earth elements are distributed widely [9]. It is well known that thermodynamic properties such as solubilities of phase equilibria and apparent molar volumes at wide temperatures are essential to explore novel methods for more effective and efficient extraction of yttrium and provide information about the ion interactions. Therefore, revealing the ion-interaction to construct a thermodynamics model at multitemperatures for the binary system ($YCl_3 + H_2O$) is of great importance.

Table 1: Comparison between the experimental ($\rho^{exp}$) and the literature values ($\rho^{lit}$) for pure water at 101.325 kPa[a].

| $T$/K | $\rho^{exp}$/g·cm$^{-3}$ | $\rho^{lit}$/g·cm$^{-3}$ [17] | $\Delta(\rho)$%[b] |
|---|---|---|---|
| 279.15 | 0.99997 | 0.99994 | 0.0030 |
| 289.15 | 0.99896 | 0.99894 | 0.0020 |
| 299.15 | 0.99680 | 0.99678 | 0.0020 |
| 309.15 | 0.99369 | 0.99369 | 0.0000 |
| 319.15 | 0.98979 | 0.98979 | 0.0000 |
| 329.15 | 0.98520 | 0.98521 | 0.0010 |
| 339.15 | 0.97999 | 0.98001 | 0.0020 |
| 349.15 | 0.97422 | 0.97424 | 0.0021 |
| 359.15 | 0.96796 | 0.96796 | 0.0000 |

[a]Standard uncertainties $u$ are $u(T) = 0.01$ K, $u(p) = 5$ kPa, and $u(\rho)$ for $\rho$ is 1.4 mg·cm$^{-3}$. [b]$\Delta(\rho)\% = 100 \times ||\rho^{exp}/\rho^{lit} - 1||$.

As to the volumetric behaviors of $YCl_3$ aqueous solutions, data reported in the literature [10, 11] were mainly focused on 298.15 K, even using the traditional pycnometric measurement method [11]. With the progress of technology, the density measurement for the aqueous solution at multiple temperatures with a vibrating-tube densimeter is more convenient and accurate than that of the pycnometric measurement [12–14]. However, up to now, there are no data reported on the apparent molar volumes at temperatures from 283.15 K to 363.15 K and 101.325 kPa. Hence, studying the volumetric properties of the binary system ($YCl_3 + H_2O$) at multitemperatures is essential for utilizing rare earth elements from geothermal water resources.

In this study, densities of $YCl_3$ aqueous solutions in the range of 0.08837–1.60639 mol·kg$^{-1}$ from 283.15 to 363.15 K and 101.325 kPa were measured by an Anton Paar digital vibrating-tube densimeter. The derived properties of apparent molar volumes ($V_\phi$), partial molar volumes ($\overline{V}_\phi$), and the coefficients of thermal expansion of the solution ($\alpha$) for $YCl_3$ aqueous solutions were obtained, and their variation tendency against temperature and molality have been discussed in detail. The Pitzer single-salt parameters of $YCl_3$ at multitemperatures and temperature-dependence equations were also obtained for the first time.

## 2. Experimental

*2.1. Materials.* Extra pure reagent $YCl_3{\cdot}6H_2O$ (CAS: 10025-94-2) in 0.99999 in the mass fraction was obtained from Aladdin Industrial Co., Ltd., without any further purification. The fresh $CO_2$-free doubly deionized water (DDW) was produced by ULUP-II-10T (Chongqing Jiuyang Co., Ltd., China), with a conductivity less than $1 \times 10^{-4}$·S·m$^{-1}$, and pH = 6.60 at 298.15 K was used in the whole study.

*2.2. Apparatus and Procedure.* Stock solutions of $YCl_3$ were prepared in the glove box filled with nitrogen gas (UNIlab Plus, MBraun, Germany), in which precise $YCl_3{\cdot}6H_2O$ and DDW were weighted using the analytical balance (Mettler Toledo, Swiss) with an uncertainty 0.2 mg, followed by vigorous shaking of the solution and then filtering through a prewashed 0.2 $\mu$m Nylon "low extractable" membrane filtering unit. The stock solution concentration of $YCl_3$ expressed in molality was determined by titrimetric analysis using mercuric nitrate with uncertainty within 0.003 in the mass fraction [15]. The concentration of $Y^{3+}$ can be obtained via ion balance and evaluated through measurement by an inductively coupled plasma optical emission spectrometer (ICP-OES, Prodigy, Leeman Corporation, America) with an uncertainty of ±0.005 in mass fraction. Moreover, all the aqueous solutions employed in experimental measurements were prepared by mass dilution of the stock solution in the nitrogen glove box and stored in glass bottles at 4°C in the refrigerator.

All the density measurements for each solution were completed within two days after the stock solution was prepared. Densities of these solutions were measured using an Anton Paar digital vibrating-tube densimeter (DMA4500, Anton Paar Co., Ltd., Austria) with an uncertainty of ±1.4 mg·cm$^{-3}$, and the densimeter has a heating attachment (Anton Paar) that keep the temperature fluctuations within ±0.01 K. Before the measurement, the densimeter was calibrated during each series of measures with dry air and freshly DDW at 293.15 K under atmospheric pressure. The results were 0.00120 g·cm$^{-3}$ for dry air and 0.99820 g·cm$^{-3}$ for DDW, which agree well with the values in the literature [16]. The reliability of the density data was ascertained by making measurements of DDW using the calibrated apparatus at a 10 K interval from 279.15 to 369.15 K and atmospheric pressure, and the density values of pure water are given in Table 1, which agree well with the data in the literature [17]. The maximum relative deviation is less than 0.003%. Finally, all measurements for the densities of $YCl_3$ (aq) were conducted at temperature intervals of 5 K from 283.15 to 363.15 K and atmospheric pressure.

## 3. Results and Discussion

*3.1. Densities.* Densities of $YCl_3$ aqueous solution against molality and temperature were determined in triplicate, and the results are given in Table 2.

Based on the experimental data in Table 2, a 3D diagram of the density for the $YCl_3$ aqueous solution against temperature and molality is shown in Figure 1. It was clearly seen that the densities of $YCl_3$ aqueous solutions decreased with the increasing temperature at constant molality.

Table 2: Densities ($\rho$) of the binary system ($YCl_3 + H_2O$) at different temperatures and molalities ($m_i$)[a].

| $T$/K | Densities $\rho$/g·cm$^{-3}$ | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | 0.00000 mol·kg$^{-1}$ | 0.08837 mol·kg$^{-1}$ | 0.31207 mol·kg$^{-1}$ | 0.52215 mol·kg$^{-1}$ | 0.72660 mol·kg$^{-1}$ | 0.93877 mol·kg$^{-1}$ | 1.16667 mol·kg$^{-1}$ | 1.38637 mol·kg$^{-1}$ | 1.60639 mol·kg$^{-1}$ |
| 283.15 | 0.99961 | 1.01559 | 1.05504 | 1.09081 | 1.12467 | 1.15939 | 1.19519 | 1.22833 | 1.26096 |
| 288.15 | 0.99902 | 1.01493 | 1.05416 | 1.08974 | 1.12345 | 1.15802 | 1.19368 | 1.22672 | 1.25924 |
| 293.15 | 0.99815 | 1.01398 | 1.05304 | 1.08848 | 1.12206 | 1.15651 | 1.19206 | 1.22501 | 1.25744 |
| 298.15 | 0.99701 | 1.01279 | 1.05172 | 1.08704 | 1.12052 | 1.15488 | 1.19033 | 1.22320 | 1.25556 |
| 303.15 | 0.99564 | 1.01138 | 1.05020 | 1.08544 | 1.11884 | 1.15312 | 1.18850 | 1.22130 | 1.25361 |
| 308.15 | 0.99404 | 1.00975 | 1.04850 | 1.08368 | 1.11702 | 1.15124 | 1.18657 | 1.21932 | 1.25157 |
| 313.15 | 0.99225 | 1.00794 | 1.04664 | 1.08177 | 1.11507 | 1.14925 | 1.18453 | 1.21725 | 1.24946 |
| 318.15 | 0.99027 | 1.00595 | 1.04462 | 1.07973 | 1.11300 | 1.14716 | 1.18241 | 1.21510 | 1.24728 |
| 323.15 | 0.98812 | 1.00379 | 1.04247 | 1.07755 | 1.11082 | 1.14496 | 1.18019 | 1.21287 | 1.24503 |
| 328.15 | 0.98580 | 1.00148 | 1.04017 | 1.07525 | 1.10852 | 1.14266 | 1.17788 | 1.21056 | 1.24270 |
| 333.15 | 0.98333 | 0.99901 | 1.03773 | 1.07284 | 1.10611 | 1.14026 | 1.17549 | 1.20817 | 1.24031 |
| 338.15 | 0.98071 | 0.99641 | 1.03517 | 1.07030 | 1.10360 | 1.13777 | 1.17301 | 1.20570 | 1.23785 |
| 343.15 | 0.97795 | 0.99367 | 1.03248 | 1.06766 | 1.10099 | 1.13519 | 1.17046 | 1.20317 | 1.23531 |
| 348.15 | 0.97506 | 0.99080 | 1.02968 | 1.06491 | 1.09829 | 1.13252 | 1.16781 | 1.20056 | 1.23268 |
| 353.15 | 0.97204 | 0.98781 | 1.02677 | 1.06206 | 1.09548 | 1.12976 | 1.16509 | 1.19787 | 1.23000 |
| 358.15 | 0.96889 | 0.98470 | 1.02374 | 1.05909 | 1.09258 | 1.12690 | 1.16229 | 1.19512 | 1.22726 |
| 363.15 | 0.96563 | 0.98149 | 1.02059 | 1.05596 | 1.08958 | 1.12396 | 1.15933 | 1.19222 | 1.22446 |

[a]Standard uncertainties $u$ are $u(T) = 0.01$ K, $u(p) = 5$ kPa, $u(m_i)$ for $YCl_3$ aqueous solution is 0.005 mol·kg$^{-1}$ and $u(\rho)$ for $\rho$ is 1.4 mg·cm$^{-3}$.

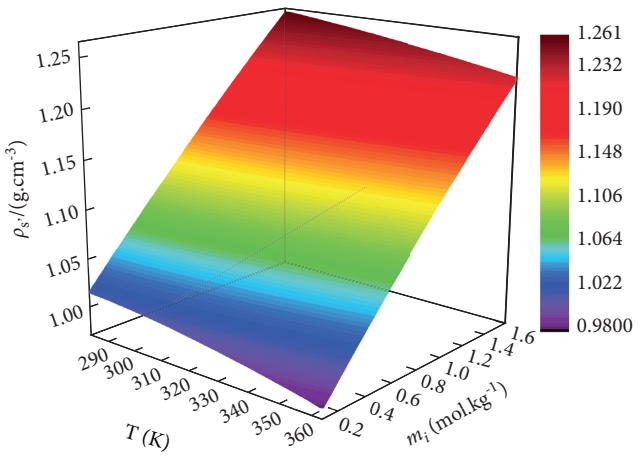


Figure 1: 3D diagram of the density of $YCl_3$ aqueous solution against temperature and molality at 101.325 kPa.

Nevertheless, at the same temperature, the density values of $YCl_3$ aqueous solutions are increased indistinctively with the increase of $YCl_3$ molality. The clear changing trend for density data may be caused by the rise in solvent-solvent and solute-solvent interactions. As the temperature increases, the volume of the aqueous solutions increases, and the density decreases. The density values at constant molality have been fitted against $(T - 273.15)$ by the least-squares method.

$$\rho = A_0 + A_1\theta + A_2\theta^2 + A_3\theta^3, \tag{1}$$

where $\rho$ is the density (g·cm$^{-3}$) of the solution; $\theta = (T - 273.15)$ K, $T$ is the absolute temperature, and $A_i$ is the empirical constant. The relevant parameters and the correlation coefficients $r$ related to the density-temperature fit obtained by applying equation (1) are given in Table S1 (Supplementary Materials). The values of the correlation coefficients ($r$) are close to 1.

According to the definition [18], the coefficient of thermal expansion of the solution is expressed with the following equations.

$$\alpha = \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_{P,m} = -\frac{1}{\rho}\left(\frac{\partial \rho}{\partial T}\right)_{P,m}, \tag{2}$$

$$\left(\frac{\partial \rho}{\partial T}\right)_{P,m} = A_1 + 2A_2\theta + 3A_3\theta^2, \tag{3}$$

$$\alpha = -\frac{1}{\rho}\left(\frac{\partial \rho}{\partial T}\right)_{P,m} = -\frac{1}{\rho}\left\{A_1 + 2A_2\theta + 3A_3\theta^2\right\}. \tag{4}$$

Based on the calculation using equation (4), the thermal expansion $\alpha$ ($K^{-1}$) values of $YCl_3$ aqueous solutions with various molalities at different temperatures were calculated and are given in Table 3. According to the calculated data, the relation diagram of the thermal expansion coefficient ($\alpha$) and the molality at temperature intervals of 5 K from 283.15 to 363.15 K is shown in Figure 2. It can be seen that the thermal expansion coefficient of $YCl_3$ aqueous solution is increased with the increase of temperature at the constant molality. With the rising of molality, the thermal expansion coefficient increased obviously at $T = (283.15–303.15)$ K, almost unchanged at $T = 308.15$ K, and then decreased slightly at $T = (313.15–363.15)$ K.

*3.2. Apparent Molar Volumes.* The apparent molar volumes can be derived from the measured densities of pure water and $YCl_3$ aqueous solutions. Their values are calculated with the following equation [19]:

$$V_\phi = \frac{1000 \times (\rho_w - \rho)}{(m_i \times \rho_w \times \rho)} + \frac{M_a}{\rho}, \tag{5}$$

where $\rho_w$ and $\rho$ are the densities (g·cm$^{-3}$) of the pure water and $YCl_3$ aqueous solutions, respectively; $m_i$ is the molality (mol·kg$^{-1}$) for $YCl_3$ aqueous solution, and $M_a$ is the molar mass (g·mol$^{-1}$) of $YCl_3$. The calculated apparent molar volumes are given in Table 4, and the 3D surfaces ($m_i$, $T$, $V_\phi$) are shown in Figure 3. It can be seen that the apparent molar volumes of $YCl_3$ aqueous solutions increased with the increase of molality at the constant temperature. With the increasing temperature, the apparent molar volumes increase when the temperature is varied within 283.15–308.15 K, and the variation tendency is opposite when the temperature is higher than 308.15 K. It can be concluded that the ionic association of yttrium and chlorine ions is strong at low temperatures [20].

*3.3. Partial Molar Volumes of Solute.* The relationship between the apparent molar volume, $V_\phi$ ($m_i$, $T$), and the partial molar volume can be expressed.

$$\overline{V}_\phi = V_\phi + m_i\left(\frac{\partial V_\phi}{\partial m_i}\right)_{P,T}, \tag{6}$$

Table 3: Coefficient of thermal expansions of the binary system ($YCl_3 + H_2O$) at different temperatures and molalities ($m_i$) at 101 kPa[a].

| $T$/K | Coefficient of thermal expansion $10^4\ \alpha/K^{-1}$ | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| | 0.08837 mol·kg$^{-1}$ | 0.31207 mol·kg$^{-1}$ | 0.52215 mol·kg$^{-1}$ | 0.72660 mol·kg$^{-1}$ | 0.93877 mol·kg$^{-1}$ | 1.16667 mol·kg$^{-1}$ | 1.38637 mol·kg$^{-1}$ | 1.60639 mol·kg$^{-1}$ |
| 283.15 | 1.19000 | 1.57546 | 1.87423 | 2.08595 | 2.28043 | 2.46108 | 2.57434 | 2.66800 |
| 288.15 | 1.66455 | 1.96031 | 2.18978 | 2.35543 | 2.50383 | 2.64060 | 2.72592 | 2.79709 |
| 293.15 | 2.12014 | 2.33183 | 2.49626 | 2.61754 | 2.72227 | 2.81766 | 2.87590 | 2.92539 |
| 298.15 | 2.55702 | 2.69014 | 2.79378 | 2.87234 | 2.93578 | 2.99226 | 3.02430 | 3.05289 |
| 303.15 | 2.97535 | 3.03540 | 3.0824 | 3.11991 | 3.14441 | 3.16446 | 3.17114 | 3.17965 |
| 308.15 | 3.37531 | 3.36766 | 3.36221 | 3.36025 | 3.34819 | 3.33425 | 3.31641 | 3.30568 |
| 313.15 | 3.75695 | 3.68700 | 3.63325 | 3.59340 | 3.54714 | 3.50169 | 3.46017 | 3.43097 |
| 318.15 | 4.12038 | 3.99348 | 3.89552 | 3.81940 | 3.74124 | 3.66677 | 3.60239 | 3.55554 |
| 323.15 | 4.46564 | 4.28705 | 4.14908 | 4.03825 | 3.93055 | 3.82952 | 3.74311 | 3.67943 |
| 328.15 | 4.79270 | 4.56780 | 4.39394 | 4.24996 | 4.1151 | 3.98995 | 3.88235 | 3.80262 |
| 333.15 | 5.10157 | 4.83572 | 4.63008 | 4.45452 | 4.29483 | 4.14809 | 4.02012 | 3.92515 |
| 338.15 | 5.39218 | 5.09077 | 4.85754 | 4.65196 | 4.46981 | 4.30392 | 4.15644 | 4.04699 |
| 343.15 | 5.66455 | 5.33297 | 5.07626 | 4.84224 | 4.63997 | 4.45747 | 4.29127 | 4.16823 |
| 348.15 | 5.91854 | 5.56223 | 5.28627 | 5.02536 | 4.80538 | 4.60880 | 4.42468 | 4.28896 |
| 353.15 | 6.15401 | 5.77844 | 5.48752 | 5.2013 | 4.96601 | 4.75782 | 4.55666 | 4.40898 |
| 358.15 | 6.37095 | 5.98170 | 5.68009 | 5.37008 | 5.12192 | 4.90462 | 4.68720 | 4.52838 |
| 363.15 | 6.56910 | 6.17194 | 5.86421 | 5.53167 | 5.27301 | 5.04955 | 4.81665 | 4.64720 |

[a]Standard uncertainties $u$ are $u(T) = 0.01$ K, $u(p) = 5$ kPa, and $u(m_i)$ for $YCl_3$ aqueous solution is 0.005 mol·kg$^{-1}$, and $u(\alpha)$ for $\alpha$ is 0.000004 K$^{-1}$.

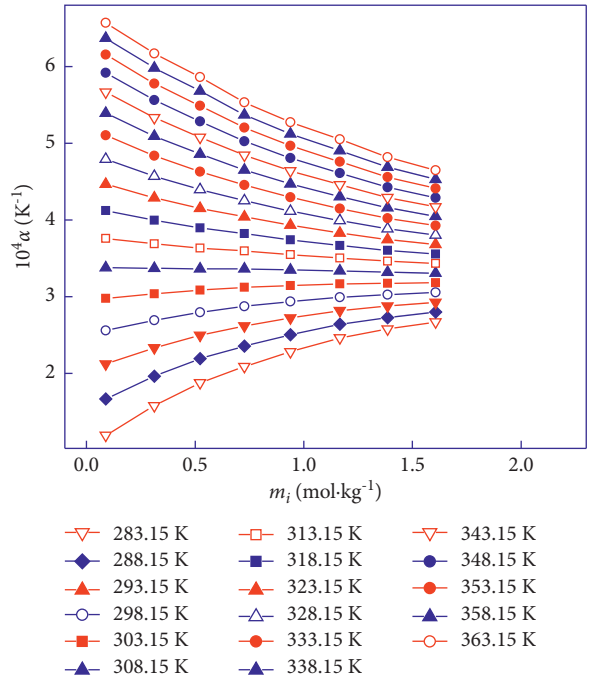


Figure 2: The coefficient of thermal expansion of $YCl_3$ aqueous solutions against temperature and molality at 101 kPa.

where $V_\phi$ refers to the apparent molar volume (cm$^3$·mol$^{-1}$), $m_i$ is the molality (mol·kg$^{-1}$) for $YCl_3$, and $(\partial V_\phi/\partial m_i)_{P,T}$ can be obtained from equations (7) and (8).

$$V_\phi = B_0 + B_1 m_i^{1/2} + B_2 m_i + B_3 m_i^{3/2} + B_4 m_i^2, \tag{7}$$

$$\left(\frac{\partial V_\phi}{\partial m_i}\right)_{P,T} = \frac{1}{2}B_1 m_i^{-1/2} + B_2 + \frac{3}{2}B_3 m_i^{1/2} + 2B_4 m_i, \tag{8}$$

where $B_i$ is the empirical constant for fitting apparent molar volume and molality at invariable temperature by the least squares, and the values of the parameters with the correlation coefficients $r$ are presented in Table S2.

Substitution of the above equation into equation (6) yields

$$\begin{aligned}\overline{V}_\phi &= V_\phi + m_i\left(\frac{\partial V_\phi}{\partial m_i}\right)_{P,T} \\ &= V_\phi + \frac{1}{2}B_1 m_i^{1/2} + B_2 m_i + \frac{3}{2}B_3 m_i^{3/2} + 2B_4 m_i^2.\end{aligned} \tag{9}$$

The calculated values for partial molar volumes of solute are given in Table 5 and shown in Figure 4. It shows that the partial molar volumes of $YCl_3$ are increased with the increase of molality at the constant temperature.

*3.4. Pitzer Parameters of YCl3.* Pitzer's electrolyte solution theory was developed based on ion-interaction and statistical mechanics, and it can accurately express the thermodynamic properties of the aqueous electrolyte solution [21]. The apparent molar volumes of $YCl_3$ were calculated using the following Pitzer equation [22].

$$\begin{aligned}V_\phi = {} & \frac{V(m_r)}{n_r} - \frac{v_W}{n_r} + \nu|z_M z_X|\left(\frac{A^\nu}{2b}\right) \\ & \cdot \ln\left\{\left(1 + bI^{1/2}\right)/\left(1 + b_r^{1/1/22}\right)\right\} + 2\nu_M \nu_X \mathrm{RT} \\ & \cdot \left\{m_i B^\nu_{MX}(m_i) - m_r B^\nu_{MX}(m_r) + \nu_M z_M C^\nu_{MX}\left(m_i^2 - m_r^2\right)\right\}.\end{aligned} \tag{10}$$

In the case of $B^\nu_{M,X}(m_i)$, the ionic strength dependence of a solution can be imposed as follows.

$$B^\nu_{\mathrm{MX}} = \beta^{(0)\nu}_{\mathrm{MX}} + \beta^{(1)\nu}_{\mathrm{MX}}\, g(\alpha\sqrt{I}), \tag{11}$$

$$g(t) = 2\left[\frac{1 - (1+t)\exp(-t)}{t^2}\right], \tag{12}$$

where $M$ and $X$ are $Y^{3+}$ and $Cl^-$, $m_i$ is the molality (mol·kg$^{-1}$) of the aqueous $YCl_3$ solutions, given in Table 4, $v_w$ is the volume of 1 kg pure water, $v_{(m_r)}$ is the volume of $m_r$, in which

Table 4: Apparent molar volumes ($V_\phi$) of the aqueous solution system ($YCl_3 + H_2O$) at different temperatures and molalities ($m_i$) and 101 kPa[a].

| $T$/K | Apparent molar volumes $V_\phi$/cm$^3$·mol$^{-1}$ | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| | 0.08837 mol·kg$^{-1}$ | 0.31207 mol·kg$^{-1}$ | 0.52215 mol·kg$^{-1}$ | 0.72660 mol·kg$^{-1}$ | 0.93877 mol·kg$^{-1}$ | 1.16667 mol·kg$^{-1}$ | 1.38637 mol·kg$^{-1}$ | 1.60639 mol·kg$^{-1}$ |
| 283.15 | 14.14715 | 16.66890 | 18.83026 | 20.51437 | 21.56110 | 23.05890 | 24.60388 | 25.77744 |
| 288.15 | 14.88817 | 17.46568 | 19.59846 | 21.22696 | 22.21798 | 23.66270 | 25.15706 | 26.29549 |
| 293.15 | 15.58570 | 18.10004 | 20.16936 | 21.75494 | 22.70508 | 24.11672 | 25.57073 | 26.68200 |
| 298.15 | 16.01782 | 18.48127 | 20.54391 | 22.09909 | 23.02785 | 24.41423 | 25.84854 | 26.93923 |
| 303.15 | 16.24606 | 18.73735 | 20.76256 | 22.31396 | 23.21884 | 24.59634 | 26.01878 | 27.09668 |
| 308.15 | 16.26898 | 18.79017 | 20.82419 | 22.37761 | 23.28182 | 24.65093 | 26.07136 | 27.15184 |
| 313.15 | 16.20441 | 18.73696 | 20.78708 | 22.33188 | 23.24453 | 24.61913 | 26.04065 | 27.12377 |
| 318.15 | 15.99441 | 18.56090 | 20.61388 | 22.17976 | 23.09626 | 24.48865 | 25.91949 | 27.01329 |
| 323.15 | 15.75454 | 18.24774 | 20.35112 | 21.93528 | 22.86700 | 24.27955 | 25.72150 | 26.83387 |
| 328.15 | 15.31196 | 17.82684 | 19.97914 | 21.59279 | 22.55071 | 23.98311 | 25.44559 | 26.57922 |
| 333.15 | 14.83975 | 17.33101 | 19.51740 | 21.16629 | 22.15345 | 23.61948 | 25.10544 | 26.26460 |
| 338.15 | 14.16310 | 16.72698 | 18.97342 | 20.65855 | 21.68353 | 23.17981 | 24.69992 | 25.88186 |
| 343.15 | 13.51306 | 16.06201 | 18.33776 | 20.07372 | 21.13109 | 22.67164 | 24.22587 | 25.44703 |
| 348.15 | 12.77401 | 15.32015 | 17.63793 | 19.42028 | 20.52537 | 22.11421 | 23.69591 | 24.97634 |
| 353.15 | 11.82582 | 14.45118 | 16.85364 | 18.69666 | 19.85027 | 21.48308 | 23.10885 | 24.43649 |
| 358.15 | 10.78264 | 13.53330 | 16.02051 | 17.90119 | 19.11908 | 20.79227 | 22.45698 | 23.83695 |
| 363.15 | 9.585831 | 12.61733 | 15.25381 | 17.06597 | 18.33323 | 20.11743 | 21.80913 | 23.19338 |

[a]Standard uncertainties $u$ are $u(T) = 0.01$ K, $u(p) = 5$ kPa, and $u(V_\phi)$ for $V_\phi$ is 0.1 cm$^3$·mol$^{-1}$. $u(m_i)$ for $YCl_3$ aqueous solution is 0.005 mol·kg$^{-1}$.

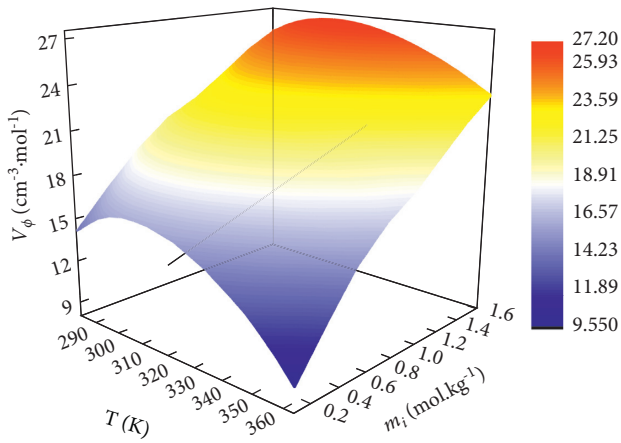


Figure 3: Apparent molar volumes of $YCl_3$ aqueous solutions against temperature and molality.

$m_r = 1.00\,\text{mol·kg}^{-1}$, $n_r = 1.00\,\text{mol}$, which is the number of moles of solute in this quantity of solution, $z_M$ and $z_X$ are the number of ionic charges of the positive and negative ion in electronic units, for $YCl_3$ ($z_M = 3$ and $z_X = 1$), $\nu_M$ and $\nu_X$ are the numbers of $M$ and $X$ ions formed by stoichiometric dissociation of one molecule of MX, and $\nu = \nu_M + \nu_X$, for $YCl_3$ ($\nu_M = 1$, $\nu_X = 3$, and $\nu = 4$), $A^v$ is the Debye–Hückel limiting law slope for the apparent molar volume [23, 24], $\alpha_{B1} = 2.0\,\text{kg}^{1/2}\text{·mol}^{1/2}$, $b = 1.2\,\text{kg}^{1/2}\text{·mol}^{-1/2}$, $I$ is the total ionic strength given by $I = (1/2)\sum m_i z_i^2$, $R = 8.314472\,\text{cm}^3\text{·MPa K}^{-1}\text{·mol}^{-1}$ is the gas constant, $T$ is a temperature in K. Pitzer's parameters $B^v_{M,X}(m_i)$ account for short-range interactions between $M$ and $X$, and the third virial coefficient $C^v_{M,X}$ means for triple ion interactions.

The Pitzer ion-interaction parameters are expressed as functions $F(i, p, T)$.

$$\beta^{(0)v}_{MX} = F(0, p, T), \tag{13}$$

$$\beta^{(1)v}_{MX} = F(1, p, T), \tag{14}$$

$$C^v_{MX} = F(2, p, T), \tag{15}$$

with $F(i, p, T)$ represented as [23]

$$F(i,p,T) = a_1 + a_2 \ln\left(\frac{T}{298.15}\right) + a_3 (T - 298.15) + \frac{a_4}{620 - T} + \frac{a_5}{T - 227}, \tag{16}$$

where $T$ is a temperature in Kelvin, $p$ is a pressure in kPa, and $a_i$ are the polynomial coefficients for equation (16). All parameters were calculated by the IAPWS-95 for the thermodynamic properties of water and the international formulation for the dielectric properties of water [25].

The available experimental data were fitted by the least-squares method to evaluate single-salt parameters by Pitzer ion-interaction theory. Based on the apparent molar volumes for ($YCl_3 + H_2O$) from 283.15 to 363.15 K in Table 4, the single-salt parameters for $YCl_3$ at each temperature were fitted based on equations (10)–(12) and are given in Table 6. The multiple correlation coefficients ($r$) were almost equal to 1, and the mean standard deviations ($\sigma$) were within ±0.0359. The temperature correlation coefficients ($a_i$) were fitted based on equations (13)–(16) and are given in Table 7. The deviation of single-salt parameters ($\beta^{(0)v}_{MX}$, $\beta^{(1)v}_{MX}$, and $C^v_{MX}$) for $YCl_3$ between all parameterization data obtained by the Pitzer model and temperature-dependence data obtained by equation (16) is within ±0.022, which indicated that the temperature-dependence equation (16) and the temperature correlation coefficients fitted in this work are reliable.

## 4. Conclusions

The volumetric properties of the ($YCl_3 + H_2O$) aqueous solution system from 283.15 K to 363.15 K at 101 kPa are investigated for the first time. Apparent molar volumes ($V_\phi$), partial molar volumes ($\overline{V}_\phi$), and the coefficient of thermal expansions of the solution ($\alpha$) of $YCl_3$ aqueous solution were derived. In addition, the Pitzer single-salt parameters ($\beta^{(0)v}_{MX}$,

Table 5: Partial molar volumes of solute ($\overline{V}_\phi$) of the binary system ($YCl_3 + H_2O$) at different temperatures and concentrations $m_i$ and 101 kPa[a].

| $T$/K | Partial molar volume, $\overline{V}_\phi$/cm$^3$·mol$^{-1}$ | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| | 0.08837 mol·kg$^{-1}$ | 0.31207 mol·kg$^{-1}$ | 0.52215 mol·kg$^{-1}$ | 0.72660 mol·kg$^{-1}$ | 0.93877 mol·kg$^{-1}$ | 1.16667 mol·kg$^{-1}$ | 1.38637 mol·kg$^{-1}$ | 1.60639 mol·kg$^{-1}$ |
| 283.15 | 16.22925 | 28.40922 | 41.30508 | 55.08407 | 70.55343 | 89.80422 | 110.78740 | 133.79942 |
| 288.15 | 17.04379 | 29.15596 | 41.88616 | 55.48636 | 70.79062 | 89.89563 | 110.76523 | 133.70611 |
| 293.15 | 17.69164 | 29.45702 | 41.81152 | 55.02301 | 69.88051 | 88.45963 | 108.75534 | 131.07495 |
| 298.15 | 18.12506 | 30.16520 | 42.90745 | 56.54599 | 71.93642 | 91.17999 | 112.21684 | 135.37522 |
| 303.15 | 18.34218 | 29.90130 | 42.00937 | 54.96909 | 69.53404 | 87.78813 | 107.74607 | 129.69940 |
| 308.15 | 18.40216 | 30.12727 | 42.40112 | 55.54831 | 70.34286 | 88.88184 | 109.16772 | 131.50221 |
| 313.15 | 18.34822 | 30.09454 | 42.39338 | 55.54248 | 70.35908 | 88.92164 | 109.22976 | 131.59189 |
| 318.15 | 18.14288 | 29.74346 | 41.82717 | 54.74579 | 69.26299 | 87.46781 | 107.37262 | 129.28087 |
| 323.15 | 17.91535 | 30.46205 | 43.79744 | 58.09613 | 74.24801 | 94.45623 | 116.53199 | 140.87366 |
| 328.15 | 17.51337 | 30.56686 | 44.50967 | 59.46830 | 76.39569 | 97.54193 | 120.63917 | 146.12243 |
| 333.15 | 17.02997 | 30.42501 | 44.82455 | 60.28481 | 77.78226 | 99.60944 | 123.42150 | 149.69102 |
| 338.15 | 16.40437 | 30.04639 | 44.68872 | 60.38437 | 78.15159 | 100.28936 | 124.43833 | 151.06723 |
| 343.15 | 15.74050 | 29.66679 | 44.68473 | 60.81131 | 79.04907 | 101.75234 | 126.48901 | 153.76331 |
| 348.15 | 15.00845 | 29.37356 | 44.94756 | 61.69617 | 80.65876 | 104.23140 | 129.88230 | 158.20052 |
| 353.15 | 14.14449 | 29.21013 | 45.57524 | 63.18244 | 83.14419 | 107.92893 | 134.90058 | 164.69806 |
| 358.15 | 13.19517 | 28.60462 | 45.28402 | 63.18822 | 83.52720 | 108.74276 | 136.18617 | 166.52731 |
| 363.15 | 12.10639 | 26.26438 | 41.23804 | 56.95956 | 74.83022 | 97.07348 | 121.18768 | 147.78314 |

[a]Standard uncertainties $u$ are $u(T) = 0.01$ K, and $u(p) = 5$ kPa. $u(m_i)$ for $YCl_3$ aqueous solution is 0.005 mol·kg$^{-1}$, and $u(\overline{V}_\phi)$ for $\overline{V}_\phi$ is 0.1 cm$^3$·mol$^{-1}$.

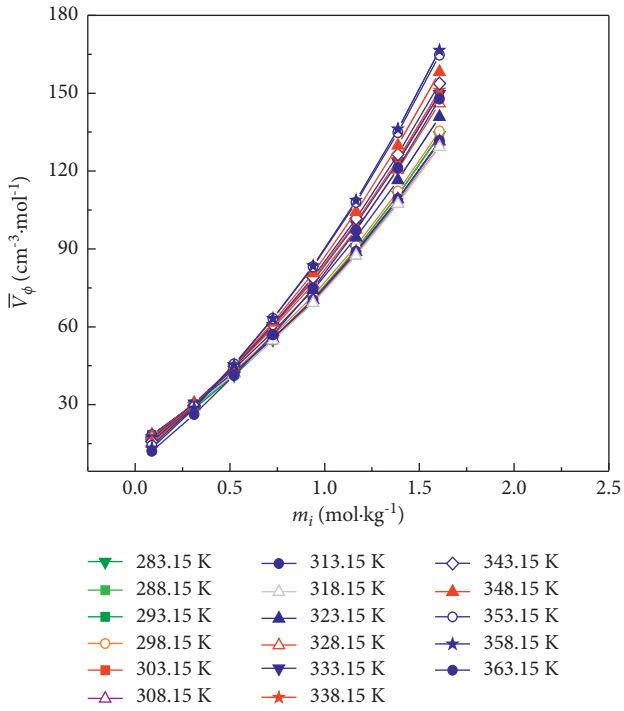


Figure 4: Partial molar volumes of the solute of $YCl_3$ aqueous solutions against temperature and molality.

Table 6: Pitzer single-salt parameters of $YCl_3$ at different temperatures[a].

| $T$/K | $10^4\beta^{(0)v}$ | $10^3\beta^{(1)v}$ | $10^5C^{(0)v}$ | $r$ | $\sigma$ |
|---|---|---|---|---|---|
| 283.15 | 2.5838 | −2.4825 | 0.0482 | 1.0000 | −0.0067 |
| 288.15 | 2.0774 | −2.2300 | 0.2620 | 1.0000 | −0.0066 |
| 293.15 | 1.7398 | −2.4362 | 0.4361 | 1.0000 | −0.0067 |
| 298.15 | 1.5464 | −2.6843 | 0.4685 | 1.0000 | −0.0060 |
| 303.15 | 1.2550 | −2.7437 | 0.6637 | 1.0000 | −0.0019 |
| 308.15 | 1.0743 | −2.8596 | 0.7479 | 1.0000 | −0.0011 |
| 313.15 | 0.9199 | −3.0562 | 0.8190 | 1.0000 | −0.0010 |
| 318.15 | 0.7690 | −3.2449 | 0.9133 | 1.0000 | −0.0039 |
| 323.15 | 0.8249 | −3.7780 | 0.7544 | 1.0000 | 0.0044 |
| 328.15 | 0.7931 | −4.0840 | 0.7145 | 1.0000 | 0.0042 |
| 333.15 | 0.7999 | −4.5500 | 0.6488 | 1.0000 | 0.0168 |
| 338.15 | 0.7361 | −4.7809 | 0.6639 | 0.9999 | 0.0128 |
| 343.15 | 0.7180 | −5.2664 | 0.6541 | 0.9999 | 0.0119 |
| 348.15 | 0.6875 | −5.7358 | 0.6704 | 0.9999 | 0.0359 |
| 353.15 | 0.6592 | −6.0450 | 0.6629 | 0.9999 | 0.0328 |
| 358.15 | 0.5329 | −6.2335 | 0.7707 | 0.9999 | 0.0329 |
| 363.15 | 0.1450 | −5.9579 | 1.1769 | 0.9999 | 0.0310 |

[a]$r$, multiple correlation coefficient; $\sigma$, mean standard deviation.

Table 7: The temperature-dependence correlation coefficients of Pitzer parameters of $YCl_3$.

| Parameters | Correlation coefficients | | | | |
|---|---|---|---|---|---|
| | $a_1$ | $a_2$ | $10^3\ a_3$ | $a_4$ | $a_5$ |
| $\beta^{(0)v}$ | 0.03237 | −0.10714 | 0.43830 | −10.07712 | −0.06494 |
| $\beta^{(1)v}$ | −0.62129 | 2.17081 | −8.73039 | 189.98924 | 2.02242 |
| $C^{(0)v}$ | −0.00371 | 0.01234 | −0.05029 | 1.15291 | 0.00969 |

$\beta^{(1)v}_{MX}$, and $C^v_{MX}$) of $YCl_3$ were parameterized from the Pitzer ion-interaction model, the temperature-dependence equation was established, and its correlation coefficients ($a_i$) were obtained for the first time.

## Data Availability

The data used to support the findings of this study are available in the article and the supplementary materials.

## Conflicts of Interest

The authors declare that they have no conflicts of interest.

## Acknowledgments

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## Supplementary Materials

The relevant parameters and the correlation coefficients $r$ related to the density-temperature fit obtained by applying equation (1) are listed in Table S1. The values of the parameters in equation (7) with the correlation coefficient ($r$) are presented in Table S2. (*Supplementary Materials*)

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