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Volumetric properties of aqueous solutions of aluminium-L-lactate

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ABSTRACT

Densities of aqueous solutions of aluminium-L-lactate <0.72 $\text{mol}\cdot\text{kg}^{-1}$, were measured at $T = 5$ K intervals, from $T = (278.15 \text{ to } 343.15)$ K. These densities served to determine the apparent molar volumes, the cubic expansion coefficients and the second derivatives of volume with respect to temperature which are interrelated with the derivatives of isobaric heat capacities with respect to pressure. Changes in the volumetric properties as a function of temperature and concentration of aluminium-L-lactate, are discussed in terms of changes in the structure of water.

1. Introduction

Aluminium-L-lactate which is produced by fermentation methods, is taking an increasing role in cosmetic, dermatological and chemical industries. Aluminium-L-lactate is a valuable non-toxic substitute in dermatological practice, by replacing aluminium acetotartrate and aluminium naphthosulphonate. On daily practice, it is an additive for toothpastes, deodorants, face and liquid creams, lipsticks, detergents, various foods and many other fine chemicals. Recently, aluminium-L-lactate is considered to be an attractive precursor for sol–gel synthesis of alumina based glasses and important component of anti-silicosis drugs (lung disease caused by inhalation of dust containing crystalline silica) [1,2].

The aluminium-lactic aquatic system is also of interest considering that the environmental toxicity of aluminium is considerably reduced by complexation and precipitation with organic acids [3–6]. To chemistry, biological aspects, structure and Al(III) speciation of organic ligands, a number of investigations was devoted [7–11]. From thermodynamic properties, there are only known the equilibrium constants of formed complexes and solubilities of aluminium-L-lactate in water, as a function of temperature [12]. Densities of aqueous solutions and derived from them thermodynamic quantities are unknown in the literature.

In this work, continuing our previous determinations of volumetric properties in systems with important organic compounds [13–16], a number of aqueous solutions of aluminium-L-lactate are considered. From determined densities, the apparent molar volumes, the cubic expansion coefficients and the change of heat capacities with pressure P (they are interrelated with the second derivatives of the volume with respect to temperature), are evaluated as a function of concentration ($m < 0.72$ $\text{mol}\cdot\text{kg}^{-1}$, to nearly saturated solutions) and temperature T. Measurements of density were performed at $T = 5$ K intervals over the $T = (278.15 \text{ to } 343.15)$ K temperature range. The reported volumetric properties of aluminium-L-lactate solutions are related to changes in the structure of water caused by dissolution aluminium-L-lactate.

2. Experimental

Aluminium-L-lactate, $Al[CH_3CH(OH)COO]_3$, (mass fraction > 0.98) was from Aldrich Chemical Company and was used without further purification. At this moment, this is the purest available commercial material, which probably includes as impurities other optical isomers of lactate and different products of the fermentation process. There is also possibility of the adsorbed from the atmosphere water in the reagent, considering its hydroscopic character. However, it was observed that this fact had a little influence on preparation of solutions and density measurements. There is no doubt that impurities are responsible for some error in density values, but it is expected that they are small enough not to influence the derived from densities the apparent molar volumes and other evaluated thermodynamic quantities.

Densities prepared by weight degassed solutions (aluminium-L-lactate + double distilled water) were determined using a Metler-Toledo DA 310 M densimeter. Calibration of the densimeter, applied procedures are similar to these described in our previous investigations [12–16]. The thermal control and stability is

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estimated to be better than $T = \pm 0.01$ K. The accuracy of our density measurements is about ± 0.0002 g·cm^{-3} and is discussed in a detail in [16]. Considering the effect of impurities, and the character of density determinations, there is difficult to determine the actual values of uncertainties and these given in table 1 should be regarded only as approximate values.

3. Results and discussion

Determined densities $d(m,T)$ of aqueous solutions of aluminium-L-lactate at given molality m, in the $T = (278.15$ to $343.15)$ K temperature range are presented in table 1. As has been shown by the first author, with a sufficient accuracy it is possible to correlate densities with the following two adjustable parameter equation,

$$d(T;\mathrm{w}) = \frac{d_{H_2O}(T)}{1 - d_{H_2O}(T)\ [\mathrm{Aw} + \mathrm{Bw}^2]}, \tag{1}$$

where w is the mass fraction of dissolved reagent and A and B are the temperature independent parameters. In the case of aluminium-L-lactate they are $A = 0.38424$ g^{-1}·cm^{-3} and $B = -0.08971$ g^{-1}·cm^{-3} with $R^2 = 0.9998$ and $\sigma(d) = 0.0004$ g·cm^{-3}.

Determined densities served to determine the apparent molar volumes $V_{2,\phi}(m,T)$ from

$$V_{2,\phi}(m,T) = \frac{M_2}{d(m,T)} + \frac{1000}{m}\left[\frac{1}{d(m,T)} - \frac{1}{d_{H_2O}(T)}\right], \tag{2}$$

where $M_2 = 294.2$ g·mol^{-1} is the molecular mass of aluminium-L-lactate and $d_{H_2O}(T)$ are densities of pure water which were taken from [17]. The apparent molar volumes of aluminium-L-lactate are presented in table 2 and at constant temperatures, they are plotted in figure 1. As can be seen, the function $V_{2,\phi}(m,T) = f(m)$ has two distinct concentration regions. In concentrated solutions, a very small change is observed. The apparent molar volumes in this region almost linearly decrease with decreasing of molality m. In dilute solutions, the values of $V_{2,\phi}(m,T)$ decrease rapidly. At constant concentration of aluminium-L-lactate, the function $V_{2,\phi}(m,T) = f(T)$ monotonically increases with temperature T (figure 2).

The cubic expansion coefficients of a solution (isobaric thermal expansibilities) are defined by

$$\alpha(m,T) = \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_{P,m} = -\left(\frac{\partial \ln d(m,T)}{\partial T}\right)_{P,m}, \tag{3}$$

and they are reported in table 3. Typical behaviour of $\alpha(m,T)$ at constant temperature is presented in figure 3 and at constant concentration in figure 4. As can be observed, the cubic expansion coefficients have the concave downward curvature in both cases and $\alpha(m,T)$ increases with increasing m and T. However, at high temperatures, the effect of concentration is very small (figure 4).

The knowledge of thermal expansion coefficients, $\alpha(m,T)$, and their derivatives with regards to temperature, $\partial\alpha(m,T)/\partial T$, is important because this permits to interrelate the volumetric and thermal properties of solutions.

From the Maxwell relation as applied to the differential of enthalpy

$$dH = C_P dT + \left[V - T\left(\frac{\partial V}{\partial T}\right)_P\right] dP, \tag{4}$$

we have

$$\left(\frac{\partial C_P}{\partial p}\right)_T = -T\left(\frac{\partial^2 V}{\partial T^2}\right)_P, \tag{5}$$

where C_P is the isobaric heat capacity of solutions. The right side of above equation can be expressed in terms of the cubic expansion coefficients and their derivatives as

TABLE 1
Densities of aqueous solutions of aluminium-L-lactate as a function of concentration and temperature.

m/m^0	$d(m,T)/\text{g·cm}^{-3}$						
Θ	5	10	15	20	25	30	35
0.0016	1.00031	1.00007	0.99946	0.99856	0.99737	0.99600	0.99437
0.0033	1.00054	1.00029	0.99969	0.99878	0.99760	0.99622	0.99459
0.0065	1.00095	1.00070	1.00009	0.99918	0.99799	0.99661	0.99498
0.0160	1.00210	1.00182	1.00121	1.00027	0.99909	0.99767	0.99604
0.0281	1.00354	1.00324	1.00260	1.00167	1.00046	0.99904	0.99740
0.0521	1.00626	1.00592	1.00525	1.00430	1.00309	1.00164	0.99999
0.0995	1.01150	1.01110	1.01037	1.00939	1.00813	1.00664	1.00496
0.1996	1.02222	1.02172	1.02089	1.01981	1.01848	1.01692	1.01517
0.3045	1.03298	1.03235	1.03143	1.03026	1.02885	1.02723	1.02541
0.4021	1.04251	1.04179	1.04077	1.03952	1.03807	1.03637	1.03451
0.5059	1.05217	1.05134	1.05024	1.04892	1.04737	1.04562	1.04370
0.5991	1.06059	1.05968	1.05850	1.05711	1.05551	1.05370	1.05173
0.7147	1.07067	1.06965	1.06838	1.06689	1.06525	1.06336	1.06135
Θ	40	45	50	55	60	65	70
0.0016	0.99255	0.99054	0.98837	0.98602	0.98353	0.98088	0.97811
0.0033	0.99276	0.99075	0.98856	0.98621	0.98372	0.98106	0.97827
0.0065	0.99314	0.99113	0.98895	0.98659	0.98409	0.98145	0.97867
0.0160	0.99421	0.99220	0.99000	0.98765	0.98514	0.98249	0.97971
0.0281	0.99556	0.99353	0.99134	0.98897	0.98648	0.98381	0.98102
0.0521	0.99812	0.99609	0.99387	0.99149	0.98897	0.98630	0.98351
0.0995	1.00306	1.00100	0.99876	0.99636	0.99382	0.99113	0.98833
0.1996	1.01323	1.01110	1.00881	1.00637	1.00379	1.00106	0.99820
0.3045	1.02341	1.02123	1.01890	1.01642	1.01380	1.01104	1.00814
0.4021	1.03244	1.03023	1.02786	1.02532	1.02268	1.01988	1.01705
0.5059	1.04159	1.03933	1.03692	1.03436	1.03167	1.02885	1.02590
0.5991	1.04959	1.04730	1.04484	1.04224	1.03953	1.03668	1.03373
0.7147	1.05914	1.05679	1.05431	1.05167	1.04893	1.04604	1.04305

$m^0 = 1$ mol·kg^{-1}; $\Theta = T/\mathrm{K} - 273.15$; $P = 101.3$ kPa.
Uncertainties U are: $U(d) = 0.00005$ g·cm^{-3}; $U(T) = 0.01$ K; $U(m) = 0.0005$ mol·kg^{-1} (see text).