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Data article

Effect of calcon carboxylic acid on association process of vanadyl sulfate in water-N, N-dimethyl formamide mixed solvents

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ABSTRACT

The complexation reaction between calcon carboxylic acid (CCA) and vanadyl sulfate was studied in water and mixed water-N, N-dimethyl formamide mixed solvents (DMF–H_2O) using conductometric measurements. The experimental data are already analyzed with the use of Fuoss–Shedlovsky technique in absence and presence of CCA. The ion-pair association (K_A), and also the standard thermodynamic parameters for association (ΔG^o_A, ΔH^o_A and ΔS^o_A) were estimated and compared in absence and presence of CCA. The main difference between Gibbs free energy of association in the presence and the case of absence of CCA indicate the value of free enthalpy of complexation ($\Delta G^\circ_{complexing}$). Walden product ($\Lambda_0 \eta_0$), hydrodynamic radii ($R_H$) and the energy of activation (E_a.) were also calculated. This work provides the suggested structure of the complex based on elemental analyses and spectral study (IR) which provide the thermodynamic results with useful discussion. CCA act as binegative tetradentate coordination.

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Specifications table

Subject area	Physical chemistry
Compounds	vanadyl sulfate, DMF and calcon carboxylic acid
Data category	Thermodynamics
Data acquisition format	Conductance data analysis to calculate thermodynamic parameters
Data type	Analyzed
Procedure	Conductance study
Data accessibility	Data is with this article

1. Rationale

Metal ions play a vital role in bio-inorganic chemistry and provide the basis of models for active sites of the biological system [1–3]. The electrolyte of vanadium battery is the core of it in energy storage and energy conversion because it is the electroactive substance which could realize energy storage. So, the critical nature of vanadium battery like charge–discharge efficiency, service life and energy density depend on the thermodynamic study of vanadyl sulfate [4–9]. (K_A) and the thermodynamic parameters are essential where these salts work well in several applications such as pharmaceutical industries and water purification …etc. Study of ion association enables us to investigate the factors affecting the thermodynamic and kinetic stability. The quality of the water in those applications which required water contain no or limited ions, including in the pharmaceutical, sea water desalination, etc. can be determined by The conductometric study [10]. Studying the conductance, viscosity, and ionic mobility (transport properties) of electrolytes in an aqueous and partially aqueous system are very useful not only explain ion-ion and ion-solvent interactions in these solutions, but also the preferential solvation of ions [11]. N, N-dimethylformamide (DMF) is called super solvent, due to its miscibility with all common polar and nonpolar solvents. It is used in the manufacture of several chemical products and intermediates as a parent substance [12]. The binary mixed solvents (DMF–H_2O) are the favorite solvents can be used for studying of ion association and ion mobility, due to the change over a wide range in its physical properties

2. Experimental procedure

2.1. Conductivity measurements of mixed solvents

The binary mixed solvents of (DMF-H_2O) with the DMF mass fractions of 0% and 50% were chosen to be the mixtures used in presence and absence of CCA and were prepared by mixing required volume of DMF and water (with error $\pm 0.02\%$). DMF percentage is equal to the term $(V_1 d_1)100$ / $(V_1 d_1 + V_2 d_2)$. Where d_1 is the density of DMF and d_2 is the density of H_2O. V_1 and V_2 are the volumes of DMF and H_2O respectively. The physical properties of the used mixed solvents at working temperatures were collected in Table 1 [13–15]. All electrical conductance carried out by the use of LF 191(Germany) conductivity meter (accuracy $\pm 0.01\%$) of a cell constant value $1 \pm 10\%\,cm^{-1}$. The cell constant was determined with potassium chloride solutions. The temperature of mixtures under study was maintained constant using a MLW 3230 ultra-thermostat with an accuracy of $\pm 0.006\,^{\circ}C$.

2.2. Chemicals

Deionized water was distilled and used in the preparation of the mixtures with a specific conductivity of $0.07\,\mu S\,cm^{-1}$ at 298.15 K. (DMF 99.9%), vanadyl sulfate trihydrate ($VOSO_4.3H_2O, \geq 99.9\%$) and calcon carboxylic acid were purchased from Sigma–Aldrich and also were used as such without further purification and potassium chloride (KCl, 99%) were supplied from Riedel-de Haën company (Germany) and also were used without further purification.