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Study on the oscillation dissolved behavior of oxysophocarpine in water

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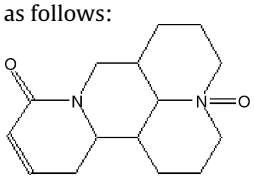
ABSTRACT

In this paper, the enthalpies of dissolution of oxysophocarpine in water were measured using a RD496-2000 Calvet microcalorimeter at 298.15 K under atmospheric pressure, showing that the dissolution process was an endothermic and exothermic oscillation behavior. A series of thermodynamics functions and the half-life were obtained by thermodynamic and kinetic methods. The results show that this work not only provide a simple method for the determination of the half-life for a drug but also offer a theoretical reference for the clinical application of resveratrol.

1. Introduction

Oxysophocarpine (chemical formula: $C_{15}H_{22}N_2O_2$, Mw. 364.36) is sophocarpine nitrogen oxide [1,2]. There are two N atoms in the molecule, one of the N atom was amide state. It normally presents as white or whitish crystalline powder without odor and with bitter taste. Its structure is as follows:



Oxysophocarpine is soluble in many organic solvents and water. Its injection always uses 0.9% sodium chloride as solvent in clinic. It is get attention and favor from the medical community for its unique effect. So it is very useful to study the solution performance and thermodynamic properties.

As the rapid development of the life sciences, the bio-thermodynamic theory and micro thermal technology also have a widely use which were applied by many scholars to study on many fields. For example: Isabel Barja et al. [3] investigated the effect of temperature on microbial activity in soils. The data from the research was very useful when studying bacterial growth thermodynamic properties in soil. Bunyan and Cunliffe [4] have used the microcalorimetry method to determine the cure reaction in some fluorinated polyether rubbers. Ingermar Wadso [5,6] has investigated of living plant materials and living cellular systems using the microcalorimetric techniques. Microcalorimetry technique was also used in biochemical area [7,8]. Yu et al. [9] have compared the micro calorimetry in some herb medicines. The results shown that the microthermal analysis method can as an effective tool to portray of herbs, combined with the reaction kinetic parameters such as ΔH can be as the indicators for drugs. Some thermal dynamic experiments have been carried out between a series of drugs and some biological macromolecules in human body by Zhang and Wang [10]. Through the analysis and summarized of experimental results they have put forward a new method using micro calorimetry technology to screen and inspection medicines. Lerman et al. [11] have also done the thermal dynamic experiment to research the interaction between the medicine and some biological macromolecules in human body by the micro calorimetry method, and have been made some progress. In our research, we have studied the dissolution behavior of drugs in reasonable solvent in which the drugs can completely dissolved. A series of thermodynamics functions and the half-life were obtained by thermodynamic and kinetic methods. The half-life was consistent to the ones from pharmacokinetics, but the method is simple. Moreover, the distribution of different systems and thermal stabilities of solutions can be generated from the ΔS during the dissolution process. So the studies of its thermodynamic functions and determination of its kinetic parameters have significant meanings on improving medicines quality and clinic applications.

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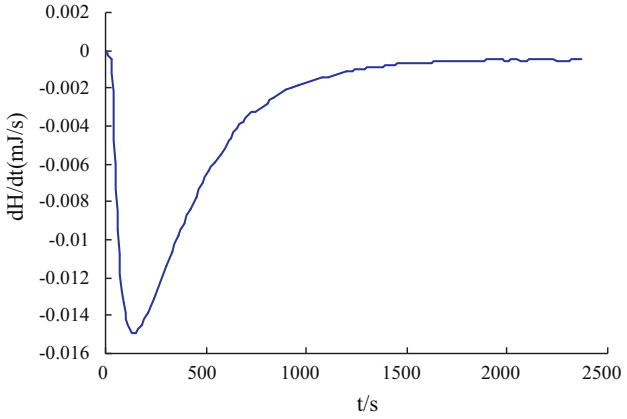

Fig. 1. The endothermic curve of dissolution process.

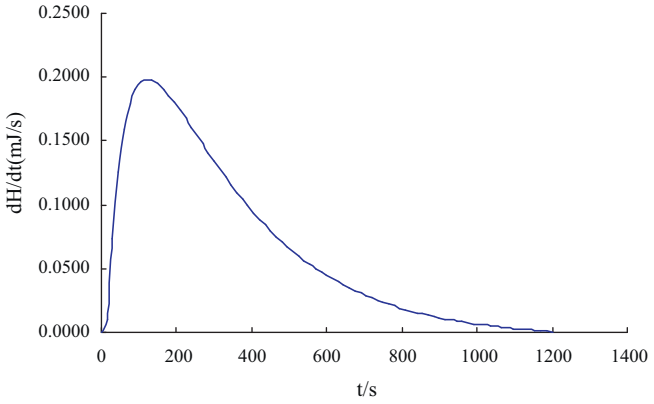

Fig. 2. The exothermic curve of dissolution process.

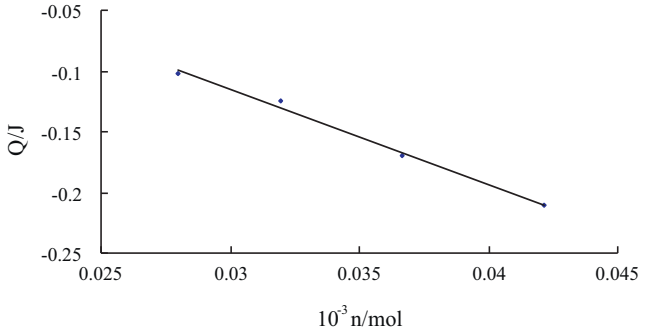

Fig. 3. Linear relationship between the heat effect (Q) and the amount of oxysophocarpine (n) in endothermic process.

2. Experimental

2.1. Materials

Oxysophocarpine was purchased from Baoji Fangsheng Biological Development Co., Ltd. (purity: >99%).

2.2. Equipment and conditions

The experiment was performed using a RD496-2000 Calvet microcalorimeter (Mianyang CAEP Thermal Analysis Instrument Company, China). The microcalorimeter was calibrated by the Joule effect, and its sensitivity was $(64.28 \pm 0.04)\,\mu V\,mW^{-1}$ at 298.15 K. The enthalpy of dissolution of KCl (spectrum purity) in distilled water (about 20 mg/2000 g) measured at 298.15 K was 17,535 kJ mol^{-1}, which was in excellent accordance with the literature value of 17,545 kJ mol^{-1} [12], showing that the device for measuring the enthalpy used in this work was reliable.

2.3. Experimental methods

The proper amount of oxysophocarpine (10.20 mg, 11.65 mg, 13.36 mg, 15.37 mg; and 21.84 mg, 25.52 mg, 29.11 mg, 33.39 mg, 41.29 mg) was dissolved in 1.50 mL of distilled water at 298.15 K under atmospheric pressure. The value of enthalpy changing of the process was detected by the RD496-2000 Calvet microcalorimeter.

3. Results and discussion

3.1. Thermochemical behaviors of dissolution of oxysophocarpine in water

It is found that the dissolution process of oxysophocarpine dissolved in distilled water is an endothermic and exothermic oscillation process. The thermodynamic parameters for two concentrations were calculated by the RD496-2000 micro-calorimeter measurements.

3.1.1. The dissolution curve

A certain mass of oxysophocarpine was dissolved in distilled water at 298.15 K. Nine concentration gradients were carried out in this experiment. The curve describing the entire dissolution process of oxysophocarpine in distilled water is shown in Figs. 1 and 2.

The dissolution is an oscillation process. It is an endothermic process when the amount of oxysophocarpine was less than 20 mg, and it is an exothermic process when the amount of oxysophocarpine was more than 20 mg. The entire process was repeated three times. The heat flow curves obtained under the same conditions overlap with each other, which indicating that the reproducibility of the tests is satisfactory.

Table 1
Dissolution enthalpy of oxysophocarpine in 1.50 mL distilled water (endothermic).

m (mg)	n ($\times 10^{-3}$ mol)	Q (J)	ΔH (kJ mol^{-1})
10.20	0.028	−0.10	−3.64
11.65	0.032	−0.12	−3.88
13.36	0.037	−0.17	−4.64
15.37	0.042	−0.21	−4.98
Average	0.035		−4.28

3.1.2. The molar enthalpy

Tables 1 and 2 show the experimental data obtained from the typical thermogram curve of the dissolution with different masses of oxysophocarpine in 1.50 mL distilled water.

As we can see in the tables, the concentration of the solvent has little influence on the values of the molar enthalpy ($\Delta_{sol}H_m$) at 298.15 K. So the average value of $\Delta_{sol}H_m$ can represent the molar

Table 2
Dissolution enthalpy of oxysophocarpine in 1.50 mL distilled water (exothermic).

m (mg)	n ($\times 10^{-3}$ mol)	Q (J)	ΔH (kJ mol^{-1})
21.84	0.060	0.59	9.83
25.52	0.070	0.68	9.71
29.11	0.080	0.86	10.75
33.39	0.092	0.98	10.65
41.29	0.113	1.25	11.06
Average	0.083		10.40

Note: n is the amount of oxysophocarpine, Q is the heat effect of the process, and $\Delta_{sol}H_m$ is the molar enthalpy.