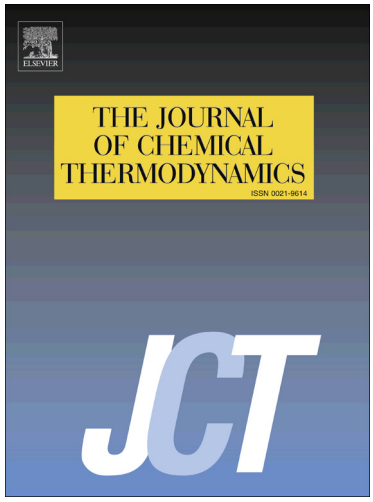

Solubility of Dihydroxylammonium 5,5'-Bistetrazole-1,1'-diolate in (formic acid, water) and their binary solvents from 298.15 K to 333.15 K at 101.1 kPa

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Solubility of Dihydroxylammonium 5,5'-Bistetrazole-1,1'-diolate in (formic acid, water) and their binary solvents from 298.15 K to 333.15 K at 101.1 kPa

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Abstract : In this study, the solubility of Dihydroxylammonium 5,5'-Bistetrazole-1,1'-diolate (TKX-50) in formic acid, water and mixed solvents (formic acid+water) were measured with the temperature ranging from 298.15 K to 333.15 K by using a laser dynamic monitoring technique at 101.1 kPa. The experimental data showed that the solubility of TKX-50 increase with the increasing temperature in all solvents and decrease with the decreasing proportion of formic acid in mixed solvents (formic acid+water) at constant temperature. The mole fraction solubility of TKX-50 in pure formic acid and pure water were correlated with the modified Apelblat equation and the van't Hoff equation, the mole fraction solubility in mixed solvents (formic acid+water) were correlated with the (CNIBS)/R-K equation, the Jouyban-Acree model, the Apelblat-Jouyban-Acree model, the van't Hoff-Jouyban-Acree model, the Sun model and the Ma model. The result showed that calculated values correlated by these models are consistent with the experimental data. The solubility of TKX-50 in mixed solvents (formic acid+water) will provide essential support for the further research of crystallization and spheroidization of TKX-50.

Keywords : Dihydroxylammonium 5,5'-Bistetrazole-1,1'-diolate Solubility spheroidization Correlation Laser dynamic monitoring technique

1 Introduction

Crystallization is not only a means of separation, but also a means of purification. It is important in the pharmaceutical industry and the fine chemicals industry[1]. Compounds which were synthesized often contain many impurities, crystallization is an essential method to separate and purify them. Additionally, crystallization plays a special role in the field of energetic materials. On the one hand, crystallization can increase the purity of explosives, generally speaking, the purity of energetic compound is a crucial factor that affecting its performance, especially on the process when explosives are tested, stored, and used[2]. On the other hand, crystallization is also an important means to control and improve the crystal morphology of energetic compound. The crystal morphology and the defect of crystal make a huge difference on the performance of explosives, for example, it affects directly the free-flowing properties; the stability; the safety and the mechanical properties of explosives. Spherical explosives are generally better in applications compared to other shapes of explosives.

Dihydroxylammonium 5,5'-Bistetrazole-1,1'-diolate (TKX-50, structure shown in Fig.1) is a new ion salt explosive of high energy and low sensitivity that was synthesized in 2012 by Niko Fischer[3]. Related performance studies showed that[3]: the theoretical maximum density of