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计算机在预测药物稳定性中的应用

魏树礼:蒲新余

北京医科大学药学院

摘要:

本文采用非恒温动力学方法对头孢唑啉的稳定性进行了研究,温度随时间连续等步增加,用计算机求解动力学方程,计 算出各步温度的速度常数与相应浓度,根据残差平方和最小原则拟合出反应的活化能,实验结果与留样观察基本一 致。

关键词: 非恒温动力学 计算机 速度常数 活化能

# APPLICATION OF COMPUTER IN PREDICTING STABILITY OF DRUGS

WEI Shu-Li and PU Xin-Yu

### Abstract:

This paper reports studies on the stability of cefazolin with nonisothermal kinetics method. The temperature was increased in consecutive equal steps. The kinetic equation was solved by computer. For > 活化能 each step, the rate constant and corresponding concentration were calculated. According to the principle of minimum sum of the squares of the difference between the experimental and the theoretical values, the corresponding activation energy is regarded as the activation energy of the reaction. The results obtained by the nonisothermal method are similar to those obtained by the long term sample observation method.

Keywords: Computer Rate constant Activation energy Nonisothermal kinetics

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