

催化、动力学与反应器

## 含氨高温液态水中苯乙腈水解反应动力学

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摘要

针对高温液态水中苯乙腈无催化水解制备苯乙酸存在反应速度慢的问题, 提出了一个含氨高温液态水中苯乙腈水解制备苯乙酰胺和苯乙酸的新方法。系统地测定了433.15 ~ 493.15 K范围内、不同氨浓度下苯乙腈及其水解的中间产物苯乙酰胺的水解反应动力学数据。从苯乙腈水解反应动力学数据可见, 苯乙酰胺的收率可从未加入氨时的26.9%增加到氨浓度为 $919.4 \text{ mg} \cdot \text{L}^{-1}$ 时的50.8%。通过动力学拟合表明, 氨的加入主要提高了苯乙腈水解产生苯乙酰胺的速度, 而对苯乙酰胺进一步水解产生苯乙酸的影响相对较小, 因而可以通过优化工艺条件得到较高的苯乙酰胺收率。同时, 无催化时一级反应动力学方程能较好地拟合苯乙腈水解反应动力学数据, 而加入氨水的情况下用二级反应动力学方程能更好地拟合动力学数据, 氨加入量为 $229.8 \text{ mg} \cdot \text{L}^{-1}$ 时苯乙腈和苯乙酰胺水解反应活化能分别降低至 $57.2 \text{ kJ} \cdot \text{mol}^{-1}$ 和 $67.7 \text{ kJ} \cdot \text{mol}^{-1}$ , 因而氨的加入有可能改变了苯乙腈水解反应的途径。新方法不仅能为苯乙酰胺和苯乙酸的绿色制备提供基础数据, 同时对提高高温液态水中有机合成反应的应用价值有一定的推动作用。

关键词

[含氨高温液态水](#) [苯乙腈](#) [苯乙酰胺](#) [苯乙酸](#) [反应动力学](#)

分类号

## Reaction kinetics of phenylacetonitrile hydrolysis in $\text{NH}_3$ -enriched high temperature liquid water

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### Abstract

In order to solve the problem of slow reaction rate for non-catalyzed hydrolysis of phenylacetonitrile in high temperature liquid water (HTLW), a new method was proposed to accelerate the reaction by the addition of  $\text{NH}_3$  to the HTLW. Hydrolysis reaction kinetics of phenylacetonitrile and phenylacetamide as its intermediate at different temperatures and ammonia concentrations was determined. From the reaction kinetics data of phenylacetonitrile hydrolysis, the yield of phenylacetamide increased from 26.9% without addition of ammonia to 50.8% at the ammonia concentration of  $919.4 \text{ mg} \cdot \text{L}^{-1}$ . From the reaction kinetics analysis, the addition of ammonia could greatly promote the reaction rate of phenylacetonitrile hydrolysis to phenylacetamide, but have relatively small impact on the hydrolysis of phenylacetamide to phenylacetic acid, indicating possibly a higher yield of phenylacetamide. For non-catalyzed hydrolysis of phenylacetonitrile in HTLW, the reaction kinetics data were in good agreement with the first order reaction kinetic equation, but second order reaction kinetic equation fitted the data well for phenylacetonitrile hydrolysis in  $\text{NH}_3$ -enriched HTLW. At the ammonia concentration of  $229.8 \text{ mg} \cdot \text{L}^{-1}$ , the activation energies for phenylacetonitrile and phenylacetamide hydrolysis lowered to  $57.2 \text{ kJ} \cdot \text{mol}^{-1}$  and  $67.7 \text{ kJ} \cdot \text{mol}^{-1}$ , respectively. All these data gave hints that the addition of ammonia to HTLW may change the pathway of phenylacetonitrile hydrolysis. This work will not only provide basic data for environmentally benign preparation of phenylacetamide and phenylacetic acid, but also improve the applicability of organic synthesis in HTLW.

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## Key words

[NH<sub>3</sub>-enriched high temperature liquid water](#) [phenylacetonitrile](#) [phenylacetamide](#) [phenylacetic acid](#)  
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