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FULL PAPERS

# 邻位吡啶自由基多通道分解反应的动力学和反应机理研究

程学礼[*, a]，李丽清[1]，李桂新[2]，赵燕云[1]，李衍飞[3]

[1]泰山学院化学系, 泰安 271021

[2]泰山学院生物工程系，泰安 271021

[2]泰山学院化学工程系， 泰安 271021

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摘要 使用Gaussian94程序包，在B3LYP/6-311++G**基组水平上，
本文对邻位吡啶自由基的多通道分解反应展开理论研究，用振动模式分析和电子布居分析阐明了反应机理，同时用动力学的方法证实了最优反应通道和主要产物。

关键词 邻位吡啶自由基, 振动模式分析, 电子布居分析, 反应速率常数

分类号

## Reaction Mechanism and Dynamic Investigations of Poly-channel Decomposition Reactions of *o*-Pyridyl Radical

CHENG Xue-Li*,[a], LI Li-Qing[1], LI Gui-Xin[2], ZHAO Yan-Yun[1], LI Yan-Fei[3]

[1]Department of Chemistry, Taishan University, Tai'an, Shandong 271021, China

[2] Department of Biological Engineering, Taishan University, Tai'an, Shandong 271021, China

[3] Department of Chemical Engineering, Taishan University, Tai'an, Shandong 271021, China

**Abstract** Utilizing Gaussian94 program package, all species involved in decomposition reactions of *o*-pyridyl radical were optimized fully at B3LYP/6-311＋＋G** level. Intrinsic reaction coordinate calculations were employed to confirm the connections of the transition states and products, and transition states were ascertained by the number of imaginary frequency (0 or 1). The reaction mechanism was elucidated by the vibrational mode analysis and electronic population analysis, and the reaction rate constants were calculated with transition state theory.

**Key words** *o*-pyridyl free radical vibrational mode analysis population analysis reaction rate constant

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通讯作者 程学礼 x_cheng@tanc.edu.cn