

研究论文

双环氧乙烷对三类亚硝胺的羟基化过程的理论研究

李澜^{1,2}, 滕国凤¹, 李宗和¹

1. 北京师范大学化学学院, 北京 100875;
2. 上海应用技术学院数理部, 上海 200235

收稿日期 2006-9-4 修回日期 网络版发布日期 2007-11-12 接受日期

摘要 采用量子化学密度泛函(DFT)方法, 在B3LYP/6-31G**水平下研究了双环氧乙烷(Dioxirane)、氧化二甲基亚硝胺(NDMA)、吡咯烷亚硝胺(NPYR)和哌啶烷亚硝胺(NPIP)中的C—H键, 三类亚硝胺化合物均形成 α -羟基化产物的反应机理. 得到三类分子的羟基化反应有 syn -和 $anti$ -两种进攻方式, 在气相和溶剂(CH_2Cl_2)中, Dioxirane氧化三类亚硝胺分子有相对低的能垒, 均容易进行 α -羟基化.

关键词 [氧化二甲基亚硝胺](#) [吡咯烷亚硝胺](#) [哌啶烷亚硝胺](#) [密度泛函方法](#) [\$\alpha\$ -羟基化](#)

分类号 [0641](#)

Theoretical Study of Hydroxylation of Nitrosodimethylamine, Nitrosopyrrolidine, and Nitrosopiperidine by Dioxirane

LI Lan^{1,2}, TENG Guo-Feng¹, LI Zong-He^{1*}

1. College of Chemistry, Beijing Normal University, Beijing 100875, China;
2. Department of Mathematics and Physics, Shanghai Institute of Applied Technology, Shanghai 200235, China

Abstract The hydroxylation reaction mechanisms of nitrosodimethylamine, nitrosopyrrolidine and nitrosopiperidine by dioxirane were theoretically investigated at the B3LYP/6-31G** level. It is found that there are two paths (separately, syn - and $anti$ -) to the hydroxylation reaction of the three nitrosoamines that have the same hydroxylation reaction mechanisms. The study of the potential surface shows that the hydroxylation of the three nitrosoamines by dioxirane has a relatively low energy barrier. The result of the theoretical study shows that the α -hydroxylation products of these nitrosoamines form easily by dioxirane.

Key words [Nitrosodimethylamine\(NDMA\)](#) [Nitrosopyrrolidine\(NPYR\)](#) [Nitrosopiperidine\(NPIP\)](#) [Density functional method](#) [\$\alpha\$ -hydroxylation](#)

DOI:

通讯作者 李宗和 lichyu_0@sohu.com

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