

## N-(芳亚甲基)芳胺Schiff碱汞化反应区域选择性研究

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**摘要** 本文用量子化学的MNDO方法对N-(苯亚甲基)苯胺、N-(苯亚甲基)-2-甲苯胺与N-(4-硝基苯亚甲基)-2-甲氧基苯胺Schiff碱汞化反应区域选择性进行了研究,结果表明,在其稳定构象下,

芳胺环上的电荷密度大于苯基亚甲基环,故汞化反应发生在芳胺环上;分子中亚胺氮原子的电荷密度最大,在汞化反应过程中,亚胺氮原子首先与醋酸汞配位,然后再进行邻位亲电进攻,生成邻位汞化产物;而在N-(苯亚甲基)-2-甲苯胺分子中,邻位甲基阻碍了亚胺氮原子与汞原子的配位作用,

故无邻位汞化产物生成。计算结果与实验结果一致,并进一步支持了已经提出的反应机理。

**关键词** [区域选择性](#) [汞化反应](#) [河南省自然科学基金资助课题](#) [N-\(芳亚甲基\)芳胺SCHIFF碱](#)

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## A study on the regio-selectivity of mercuration of schiff bases of N-(arylmethylene)arylamines

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**Abstract** MNDO method was applied to the study of the regio-selectivity of mercuration of N-(benzylidene) aniline, N-(benzylidene)-2-toluidine and N-(4- nitrobenzylidene)-2-methoxy-aniline. The results obtained disclosed that the electron densities on the N-phenyl ring in the stable conformations are larger than those on the C-phenyl ring. Therefore, the mercuration occurs in N-phenyl ring rather than in C-phenyl ring. The electron population on the imino-nitrogen atom is the largest, thus the mercuric acetate should first coordinate with imino-nitrogen atom in the process of the reaction and then subsequent electrophilic substitution takes place in the ortho-position of the N-phenyl ring. However, in the stable conformation of N-(benzylidene)-2-toluidine, the o-methyl group blocks the way of the imino-nitrogen atom to coordinate with mercuric acetate, the mercury atom can not be directed into the ortho-position of the N-phenyl ring and thus only para-mercuration product is formed. The calculated results are consistent with those of the experimental and further support the mechanism proposed previously.

**Key words** [REGIOSELECTIVITY](#)

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