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Nitrolysis Mechanism of 1,3,5,7-Tetraacetyl-1,3,5,7-tetrazacyclooctane

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Abstract: In order to provide better guidance to the preparation of HMX by nitrolysis of 1,3,5,7-tetraacetyl-1,3,5,7-tetrazacyclooctane (TAT), the nitrolysis mechanism was investigated. Two byproducts 1,5-diacetyl-3,7-dinitro-1,3,5,7-tetrazacyclooctane (DADN) and 1-acetyl-3,5,7-trinitro-1,3,5,7-tetrazacyclooctane (SEX) were obtained by flash column chromatography and were indentified by ^{1}H NMR, FTIR and elementary analysis. The results reveal that TAT is nitrated in succession to form HMX, and the order of the reaction rate is $k_2 > k_1$, $k_2 > k_3 > k_4$.

Key words: orgamic chemistry; dinitrogen pentoxide(N_2O_5); 1,3,5,7-tetraacetyl-1,3,5,7-tetrazacyclooctane (TAT); HMX; 1,5-diacetyl-3,7-dinitro-1,3,5,7-tetrazacyclooctane (DADN); 1-acetyl-3,5,7-trinitro-1,3,5,7-tetrazacyclooctane (SEX); nitrolysis
CLC number: TJ55; O62 **Document code**: A **DOI**: 10.3969/j.issn.1006-9941.2012.04.010

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为了更好更快地报道含能材料领域的最新成果和进展,为本领域的研究者赢得在科学共同体中的学术优先权,《含能材料》编辑部鼓励广大研究者提供"研究快报"稿件。

研究快报应简要报道含能材料领域的前沿性、创新性研究成果。编辑部鼓励研究者发表新思想、新观点、新原理和新发现,支持报道阶段性的重要研究成果的简要情况。凡被本刊以快报形式刊登的研究成果,编辑部按照国际学术惯例,允许作者以完整的研究论文的形式发表在其他国内外刊物上。

研究快报的来稿要求与投本刊的研究论文基本一致。作者投稿时需要对文章的学术价值和创新性进行简要说明。来稿要求关键数据齐备,结论明确,背景、方法和过程的介绍从简。来稿需有中英文摘要、关键词、作者简介、基金项目等信息。全文篇幅在2页(约4000字)以内。

本刊对研究快报将即审即发,以提高时效性。对有基金支持的英文稿件择优录用。

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