

油品与添加剂

## 相转移催化法合成十六烷值改进剂4,4-二硝基戊酸甲酯

谢国华 战风涛 朱丽萍 吕志凤

石油大学

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**摘要** 用二硝基乙烷钾和丙烯酸甲酯在相转移催化剂的作用下,通过Michael加成反应合成4,4-二硝基戊酸甲酯,产物可用作柴油十六烷值改进剂。研究了相转移催化剂的种类及反应条件对产物收率的影响,并用红外光谱和质谱对产物进行了鉴定。较适宜的反应条件为:以0.25%~0.5%(相对二硝基乙烷钾的摩尔数)的四丁基氯化铵作催化剂,  $m(\text{二硝基乙烷钾}):m(\text{丙烯酸甲酯})=1:3$ ,  $m(\text{二硝基乙烷钾}):m(\text{水})=1:20$ , 反应温度25~45℃, 反应时间0.5小时, 产物收率可达80.0%, 纯度达到99.9%

**关键词** [十六烷值改进剂](#) [相转移催化](#) [合成](#) [四丁基氯化铵](#)

分类号

## Synthesis of Novel Cetane Number Improver Methyl 4,4-dinitropentanoate by Phase Transfer Catalysis

### Abstract

The methyl 4, 4-dinitropentanoate has been synthesized by the Michael addition of potassium dinitroethane with methyl acrylate in the presence of tetrabutyl ammonium chloride as phase-transfer catalyst (PTC) and the compound could be used as cetane number improver in diesel fuels. The IR and GC/MS were used to identify the structure of the compound, and some factors to influence the yield were studied. Several PTCs were investigated, but only tetrabutyl ammonium chloride did the preferable yields. The addition product (methyl 4,4-dinitropentanoate) was obtained at 25~45℃ for about 0.5 hours and the ratio of potassium dinitroethane to methyl acrylate in 1:3(mol) and the ratio of water to potassium dinitroethane in 20:1, and the yield could be reached to 80%, while the tetrabutyl ammonium chloride was 0.25%~0.5% (based on potassium dinitroethane).

**Key words** [cetane number improver](#) [phase transfer catalysis](#) [synthesis](#) [tetrabutyl ammonium chloride](#)

DOI:

通讯作者 谢国华 [xieyunq@tom.com](mailto:xieyunq@tom.com)

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