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A Theoretical and Experimental Study on the Effect of Cationic Moiety of Quaternary Ammonium Tribromides in Bromination Reactions

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Abstract

Attempt has been made to explain why different aliphatic quaternary ammonium tribromides (QATBs) show different levels of efficiency in bromination reactions. For this study, tetrabutyl ammonium tribromide (TBATB, $[N(C_4H_9)_4]Br_3$), and cetyl trimethyl ammonium tribromide (CTMATB, $[N(CH_3)_3C_{16}H_{33}]Br_3$) were used as representative examples. UV-Vis Spectroscopic method was employed to measure the thermodynamic parameters of the reactions. Influence of quaternary ammonium cation on tribromide (Br_3^-) performance was assessed with the aid of Density Functional Theory (B3LYP/6-311++G(d,p)) by determining the dissociation energy of the QATBs, energies of pairs of their frontier orbitals, which are HOMO and LUMO and calculation of dipole moments.

Keywords: Quaternary ammonium tribromides, UV-Vis Spectroscopic method, frontier orbitals, B3LYP/6-311++G(d,p)

1. Introduction

Quaternary Ammonium Tribromides (QATBs) are known as alternatives to molecular bromine and have been seen to act as highly efficient reagents in numerous organic transformations.¹⁻⁴ QATBs have been playing a vital role in bromination reactions since more than half a century now. Numerous environmentally benign methods have been developed for bromination of organic substrates using QATBs which have proved to be successful.⁵⁻⁸

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