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PROTON AFFINITY AND PROTONATION SITES IN P-NITROANILINE
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Abstract

We present a study of the effect that substituents with competitive inductive properties have on the reactivity of the aromatic ring. As specific case, we studied the gas phase protonation of paranitroaniline (PNA) using Density Functional Theory methods (DFT) and Moller Plesset second order perturbation Theory (MP2). The joint effect of the substituents yields relative stabilities on the protonated species that follow the trend nitro group > amino group > ortho carbon > para carbon > meta carbon > ipso carbon (positions relative to the amino group).

Keywords

Proton affinity, reactivity in aromatic rings, competitive inductive effects, p-Nitroaniline.

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