

Competing Reactions in Ozonation of Polycyclic Aromatic Hydrocarbons

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Anthracene undergoes attack by ozone predominantly at the atoms of lowest atom or para localization energy. This occurs by two competing routes. The first involves one mole-equivalent of ozone and the formation of a trans-annular ozonide which affords either anthraquinone or ring rupture products, depending on the solvent and work-up conditions. The second route involves three mole-equivalents of ozone and results in anthraquinone and three mole-equivalents of molecular oxygen. Initial bond attack is a minor reaction.

Benz[a]anthracene undergoes the same competing reactions; bond attack competes more favorably than with anthracene, although it does not predominate over atom attack. The solvent appears to play a role in the competition.

From a survey of the recent literature regarding the ozonation of various polycyclic aromatic hydrocarbons, it can be seen that if the hydrocarbons are arranged in the order of decreasing differences between bond and atom localization energies, those in the upper part of the list undergo predominant atom attack, whereas those in the lower part of the list undergo predominant bond attack by ozone.

MO Studies of Aromatic Systems

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This paper will discuss the problem of aromaticity, and the calculation of physical and chemical properties of aromatic systems by quantum mechanical methods. A new approach based on the use of various modifications of the Pople SCF MO method will be described.