Theoretical Study of the Kolbe-Schmitt Reaction Mechanism

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A theoretical study of the Kolbe-Schmitt reaction mechanism, performed using a DFT method, reveals that the reaction between sodium phenoxide and carbon dioxide proceeds with the formation of three transition states and three intermediates. In the first step of the reaction, a polarized O-Na bond of sodium phenoxide is attacked by the carbon dioxide molecule, and the intermediate NaPh-CO_2 complex is formed. In the next step of the reaction the electrophilic carbon atom attacks the ring primarily at the ortho position, thus forming two new intermediates. The final product, sodium salicylate, is formed by a 1,3-proton shift from C to O atom. The mechanism agrees with the experimental data related to the Kolbe-Schmitt reaction.

Key words: Sodium Phenoxide; Carbon Dioxide; Density Functional Calculations.