Transesterification of Diethyl Carbonate with Methanol Catalyzed by Sodium Methoxide

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Abstract—The mechanism of sodium methoxide-catalyzed transesterification of diethyl carbonate with methanol to dimethyl carbonate has been studied by DFT quantum chemical calculations using B3LYP functional. Ethoxy groups in the substrate are replaced successively through four-coordinate carbon intermediates which undergo β-decomposition. Sodium methoxide with carbonates forms pre-reaction complexes where the sodium cation is coordinated to the carbonate fragment. These complexes are characterized by enhanced electron-donating power of the methoxy fragment and increased electron-withdrawing power of the carbonate fragment, which favors the transesterification process.

Keywords: dimethyl carbonate, transesterification, sodium methoxide, catalysis, mechanism.

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