Electroreduction of Organic Compounds, 35 [1]. Quantum Chemical Calculations of Reaction Pathways for the Cathodic Dehalogenation of Chlorodibenzofurans and Oligochlorobenzenes

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Quantum chemical (DFT) calculations on the course of the electroreductive carboxylation of chloroarenes were performed. An explanation for the extraordinary behaviour of 2-chlorodibenzofuran (**2**) as compared with the corresponding 1-chloro, 3-chloro and 4-chloro derivatives was sought for and was found in the particular reaction coordinate of **2** and in the SOMO spin density distributions of the four isomers. In the same way, the regioselectivity in the formation of dicarboxylic acids from hexachloro- and 1,2,4,5-tetrachlorobenzene was investigated by DFT-MO calculations and was shown to be due to orbital effects besides steric hindrance.

Key words: Cathodic Dehalogenation, Reaction Mechanism, DFT-MO Calculations