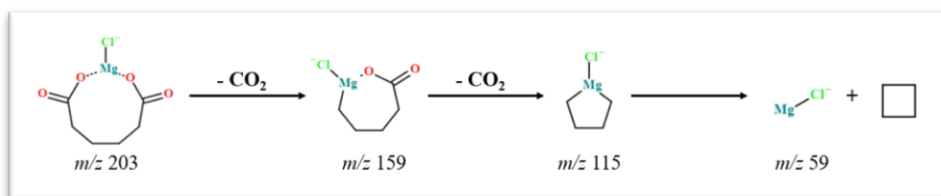


Reaction model for the formation of the new C-C bond by magnesium promoted decarboxylation of the Adipic Acid – a mass spectrometry study.

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The mixture of adipic acid and magnesium chloride was used to study the gas-phase reactivity of negatively charged bicarboxylate-magnesium chloride complex ions in the mass spectrometer. The kinetic properties and detailed reaction mechanism was investigated by both: the pressure controlled ER-CID experimental technique and DFT methods. It has been shown, that bicarboxylate-metal complexes can undergo under kinetic control the sequential decarboxylation leading to the formation of the new C-C bond within the cyclobutane. A very first step of the reaction, the loss of the neutral CO_2 leads to the formation of an intermediate structure in which the carbon-magnesium bond is essential in organometallic cyclic geometry form. The second decarboxylation leads to next intermediate in which the $-\text{C-Mg}(\text{Cl})-\text{C}-$ binding motif play a key role, from which at the very end of the mechanism the loss of MgCl promotes the new carbon-carbon bond stabilization within the cyclobutane structure. In this project, the modified mass spectrometry instrumentation with upgraded gas inlet system was used to measure the activation barriers of each reaction step. The differences in adipic acid decarboxylation abilities with and without a second, catalytic body was also analyzed. Ultimately, the comprehensive reaction mechanism was proposed by utilization of the DFT-derived reaction model and experimental data.