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Thermal transformation of carboxylic acids on nanoscale oxides seen by TPD-MS, FTIR and quantum chemical methods

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In one of the recent reviews, it has been shown that effective biomass conversion requires the integration of biochemical and thermochemical methods [1]. A catalytic pyrolysis is a promising tool for further upgrading of pyrolysis oils components to the value-added fuels and chemicals [2]. The identification of reaction products and the understanding of the mechanisms of thermal decomposition of pyrolysis oils components on the surface of potential catalysts are essential for the development of efficient biomass conversion technologies. A full understanding of the mechanisms of surface-assisted catalytic transformations has proven to be difficult even for such well-studied biomass components as carboxylic acids. Carboxylic acids of different structures can be produced on an industrial scale from non-food raw materials of the second generation by using pyrolysis, chemical and biochemical catalysis [3,4]. At the moment, some of them are considered as key-building platforms in biomass conversion technologies [3,4]. The upgrading of bio-derived carboxylic acids is a very important task because many of them are key building blocks of important polymers.
In this work, the most important experimental methods of physical organic chemistry for establishing mechanisms of catalytic reactions of carboxylic acids were applied: 1) kinetic study; 2) analysis of substituent effects by using a modified Taft equation lgk/ko=lg(B/2.3lgB)·ΔTmax/To max [5] and 3) linear free energy relationships (LFERs). The non-isothermal kinetic parameters of decomposition of the reacting series of fatty acids on the nanoscale oxides surfaces, such as the temperature of the maximum desorption rate Tmax, the reaction order n, the activation energy E≠, the pre-exponential factor ν0 and activation entropy dS≠, were calculated from TPD MS data. The thermal evolution of fatty acids surface complexes was investigated by using FTIR spectroscopy and quantum chemical methods.

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Primary authors: KULIK, Tetiana (Chuiko Institute of Surface Chemistry of NAS of Ukraine); Dr PALIANYTSIA, Borys (Chuiko Institute of Surface Chemistry, National Academy of Sciences of Ukraine); Dr ILCHENKO, Mykola (Institute of Molecular Biology and Genetics of National Academy of Sciences of Ukraine); Dr TELBIZ, German (L.V. Pisarzhevskii Institute of Physical Chemistry of the National Academy of Sciences of Ukraine); Prof. LARSSON, Mats (Stockholm University, AlbaNova University Center, Department of Physics)

Presenter: KULIK, Tetiana (Chuiko Institute of Surface Chemistry of NAS of Ukraine)

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