One-pass CH_4 carbonylation with CO_2 to acetic acid over CeO_2 -ZnO/MMT: A mechanistic comprehension

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Conversion of CH_4 and CO_2 into value-added products has vital environmental and economic importance. Their direct conversion to acetic acid is challenging due to high activation energy. Therefore, kinetic and mechanistic fundamentals must be understood. As such, co-conversion of CH_4 and CO_2 to acetic acid reaction was carried out over CeO_2 -ZnO/MMT catalyst and mechanism was tracked by quick solid state NMR, TGA, and FTIR. The reaction mimics Langmuir-Hinshelwood kind of mechanism over dual active site catalyst with reactants non-competing, preferential adsorption. The results display Zn-COOH formation is much easier, than Ce-COOH, which is confirmed to be accurate by DFT calculations. This work was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of education. (NRF-2017R1D1A1B03036324).