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Hydrogenation of Dicarboxylic Acid Diesters to Corresponding Dialdehydes over ZrO₂ Based Catalysts (Part 2) Analysis of Catalyst Surface Using Diffuse Reflectance FT-IR and CP/MAS ¹³C-NMR Spectroscopy

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The adsorption species on ZrO₂ or Cr-ZrO₂ catalyst in the hydrogenation of dimethyl benzenedicarboxylates as well as benzoic acid were characterized by diffuse reflectance FT-IR and CP/MAS ¹³C-NMR spectroscopy. Benzoic acid and dimethyl terephthalate were adsorbed as the monocarboxylate species with weak bonding to the catalyst with lower polarization at a carbonyl group similar to that of free benzoic acid. In contrast, dimethyl phthalate was adsorbed only as the dicarboxylate species. Dimethyl isophthalate was adsorbed as both mono- and dicarboxylic species. Formation of dicarboxylate adsorption species will greatly hinder the hydrogenation of dimethyl benzenedicarboxylates. In addition, the methoxycarbonyl group was more favorable for the adsorption to form the carboxylic active species than the formyl group in the interaction of Cr-ZrO₂ catalyst with terephthalaldehydic acid methyl ester. A reaction mechanism for the hydrogenation is also proposed.

Keywords: [Diester hydrogenation](#), [Zirconia catalyst](#), [FT-IR](#), [Reaction mechanism](#), [Magic angle spinning NMR](#), [Dialdehyde](#)



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