The Activity of Bimetallic Pdir/C and Monometallic Ir/C Catalysts for the Conversion of Furfural via its Hydrogenation and Acetalization

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Furfural (FU) derived from sustainable lignocellulosic biomass is a green platform molecule for synthesis of chemicals and fuels. Furfuryl alcohol (FA) produced by FU hydrogenation can be used for fine chemicals, lubricants, polymers, and pharmaceuticals. The acetal (AC) formed by acetalization of FU with alcohol solvent is seen as promising Diesel fuel additive. Here, the bimetallic PdIr/C catalysts with various Pd:Ir ratios and Pd–Ir structures formed by "water-in-oil" microemulsion method on mesoporous Vulcan carbon support. They were applied for liquid phase FU conversion in batch reactor in 2-propanol solvent under 6 bars of H₂ at only 35 °C. The monometallic Pd/C and Ir/C were also tested. The role of Ir addition is examined. The concurrent reactions of hydrogenation and acetalization are analyzed [1].

The monometallic Ir/C with a surface composed of only oxidized Ir presented exceptional selectivity >99% towards furfural diisopropyl acetal (AC) while FA was not formed at all. The formation of active sites in the Ir/C catalyst by initial hydrogen activation was necessary for acetalization to occur. The AC was not converted to ether (subsequent product), contrary to what was observed when the Pd/C catalyst was used.

The bimetallic PdIr/C catalysts with the specific composition of 15 or 26 mol% of Ir and 85% or 74 mol% of Pd, respectively, with mostly alloyed PdIr nanoparticles and their surface enriched in Pd, offered the highest TOF and FA selectivity (up to S=85%) much higher than observed for the Pd/C (S=57%). It was correlated with the lowest H₂ sorption heat, i.e., the weakest H₂ adsorption strength on the catalysts surface. The PdIr/C with 5 or 9 mol% of Ir, with the surface enriched in Ir, revealed stronger H₂ adsorption strength and activated the acetalization path much stronger as well. The electron deficient sites of IrO_x (after hydrogen activation) seems to catalyze acetalization. On the other side, when the catalysts with a lower fraction of oxidized Ir and with the alloyed structure of PdIr were used, the FU hydrogenation was more pronounced. The PdIr/C catalysts were generally more selective towards FA than the monometallic Pd/C.





Fig.1. The H₂ sorption heat (Q) and TOF (a) against Ir content in PdIr/C catalysts; FA selectivity (b), and AC selectivity (c) against FU conversion (C_{FU}).

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