

Surface chemistry of selected supported metallocene catalysts studied by DR-FTIR, CPMAS NMR, and XPS techniques. Atiqullah, M.; Akhtar, M. N.; Faiz, M.; Moman, A.; Abu-Raqabah, A. H.; Khan, J. H.; Wazeer, M. I.. Center for Refining & Petrochemicals, Research Institute, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia. Surface and Interface Analysis (2006), 38(10), 1319-1327

Abstract

Two supported metallocene catalysts (CS 1: PQ 3030/MAO/Cp₂ZrCl₂ and CS 2: PQ 3030-BuGeCl₃/MAO/Cp₂ZrCl₂) were prepd. by sequentially loading MAO and Cp₂ZrCl₂ on partially dehydroxylated silica PQ 3030. In catalyst CS 2, nBuGeCl₃ was used to functionalize the silica. These catalysts were characterized by DR-FTIR spectroscopy, CPMAS NMR spectroscopy, and XPS. Their catalytic performance was evaluated by polymg. ethylene using the MAO cocatalyst and characterizing the resulting polymers by GPC. Both catalysts produced two metallocenium cations (Cation 1: [Cp₂ZrCl]⁺ and Cation 2: [Cp₂ZrMe]⁺) with comparable equil. concns. and showed varying solid-state electronic environments. The modified supports (PQ 3030/MAO and PQ 3030-BuGeCl₃/MAO) acted as weakly coordinating polyanions and stabilized the above cations. BuGeCl₃ did not affect the solid-state electronic environment. However, it increased the surface cocatalyst to catalyst molar ratio (Al:Zr), acted as a spacer, increased catalyst activity, and enhanced chain-transfer reactions. The sep. fed MAO cocatalyst shifted the equil. between Cation 1 and Cation 2 toward the right. Consequently, more Cation 2 was generated, which acted as the effective and active single-site catalytic species producing monomodal PDI.