Spectroscopic investigation of a chromium-pyrrolyl ethene trimerization catalyst

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Linear alpha olefins (LAOs) enjoy a wide range of applications in modern society. Shorter LAOs (C₄ - C₈) are employed as comonomers in the production of linear low-density polyethylene (LLDPE), whereas longer LAOs (C₁₀+) are used in the production of surfactants and detergents. LAOs are industrially produced via catalysts which operate in a non-selective fashion, giving rise to a statistical product distribution. However, market demand for shorter LAOs is growing rapidly due to an increasing demand for LLDPE. As a result, companies are commercializing chromium catalysts which are capable of selectively oligomerizing ethene to form 1-hexene.

One of the first systems to be commercialized was developed by Chevron Phillips Chemical in Qatar in 2003. Their system consists of Cr(III) 2-ethylhexanoate, a pyrrole ligand and large quantities of alkylaluminium reagents. Despite its successful commercialization, the structure and oxidation state of the activated catalyst remains subject to debate.

In this presentation, we will be giving an overview of a spectroscopic investigation (XAS, EPR and UV-Vis) of the Chevron Phillips Chemical system. It will be shown that the Cr(III) precursor is trinuclear in nature, instead of the assumed mononuclear structure. Upon activation of this Cr(III) precursor, various Cr(I) and Cr(II) intermediates are identified. Employing aromatic solvents during the activation leads to an increased Cr(I) concentration; this is due to formation of bis(arene)Cr(I) complexes and leads to deactivation of the catalyst. Catalytic studies allow us to exclude some of the observed Cr(I) and Cr(II) intermediates as being the active species in this catalytic system.


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