Polymerization and Transalkylation Reactions of Toluene on Cu(II)-Montmorillonite

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Abstract: Products resulting from the reaction of toluene with Cu(II)-montmorillonite were analyzed using GC/MS, HPLC/MS, GPC, and FTIR methods. Numerous oligomers of toluene were observed, extending at least as high as the resolution limit (1500 g/mol) of the GPC column. The FTIR spectrum of the nonvolatile components of the extract was very similar to that of liquid toluene. GC/MS data on the volatile components revealed dimers, trimers, and a multitude of transmethylated products. Oligomerization proceeded via both ring-ring (i.e., polyphenyl) and ring-methyl linkages. The primary transmethylated products were tert-butylbenzene and isopropylxylene, indicating a competition between ring-and side-chain methylations. The side-chain substitutions cannot be explained in terms of the aromatic radical cation intermediate which typically forms in arene/clay reactions. A consideration of alkylbenzene reactions observed in various other media suggests that the present transmethylation reactions occur via a benzyl cation intermediate.

Key Words: FTIR, GC/MS • Gel permeation chromatography • Montmorillonite • Polymerization • Toluene • Transalkylation

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