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Metallation of Mesitylene by Organolithium Compounds in the Presence of Lithium Polyether Alkoxides

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Abstract: The catalytic effect of polyether alkoxides (PEAs) on the activity Of organolithium compounds as a metallating agent studied. The sites of metallation as mono, di, tri, and gem metallation at three different benzylic positions were investigated in terms of relative yield by using gas chromatography-mass spectroscopy (GC-MS couple) techniques. The yield of the trimetallated (1,3,5-metallated) mesitylene was optimized by improving the metallation conditions. Special attention was paid to the effect of metal type, alkoxide structure, solvent polarity, temperature and also relative mole ratios of was reactants such as alkoxide to mesitylene and n-butyllithium to mesitylene on metallation reactions. It was found that when the amount of n-butyllithium increases, and the amount of polyetheralkoxide decreases, the extent of metallation increases. Moreover, the yield of the metallation of mesitylene can be increased if the reaction is carried out at higher temperatures by using n-butyllithium (n-BuLi) and sodium 2-methoxyethoxide (NaOEM) in tetrahydrofuran with a mole ratio NaOEM:n-BuLi:Mesitylene= 3:6.33:1.

Key Words: Metallation of mesitylene, Polyether alkoxide, Organolithium compounds, Regioselectivity.

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