Reactivity and Regioselectivity in the Heck Reaction - A Hammett Study of 4-Substituted Styrenes - DTU Orbit (03/01/2019)

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The regioselectivity in the cationic Heck reaction of 4-substituted styrenes was addressed by a Hammett study. In this branching reaction, plots based on the substrate reactivity did not give meaningful data, whereas the product distribution was variable due to differing preferences for further substitution under the reaction conditions and, thus, unsuitable for Hammett plots. Mechanistically meaningful graphs were obtained by combination of the measured initial branching ratio with the approximately constant substrate reactivity. For the alpha-substitution a clear Hammett relation is observed, whereas beta-substitution does not depend on electronic effects. This implies that, for alpha-substitution, the slow step of the addition is an electrophilic attack by Pd(II) on the double bond, followed by a rapid migratory insertion.

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