

Allylic C—H alkylation of unactivated α -olefins

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Reactions that proceed via serial ligand catalysis mechanisms require a delicate interplay of several kinetically labile ligands. We report an investigation of the disruption of this balance and its ramifications in the case of allylic C-H alkylation. Overly competitive ligands, like the DMSO required for functionalization, were found to disrupt formation of the Pd/bis-sulfoxide catalyst required for C-H cleavage and inhibit the catalytic cycle. Insights derived from this study were applied to identify an alternate bis-sulfoxide ligand that could better compete with DMSO for binding to Pd. This has led to the development of the first intermolecular allylic C-H alkylation of unactivated α -olefins.

