Bismuth-catalysed hydroalkylation of styrene with acetylacetone – an unexpected mechanism

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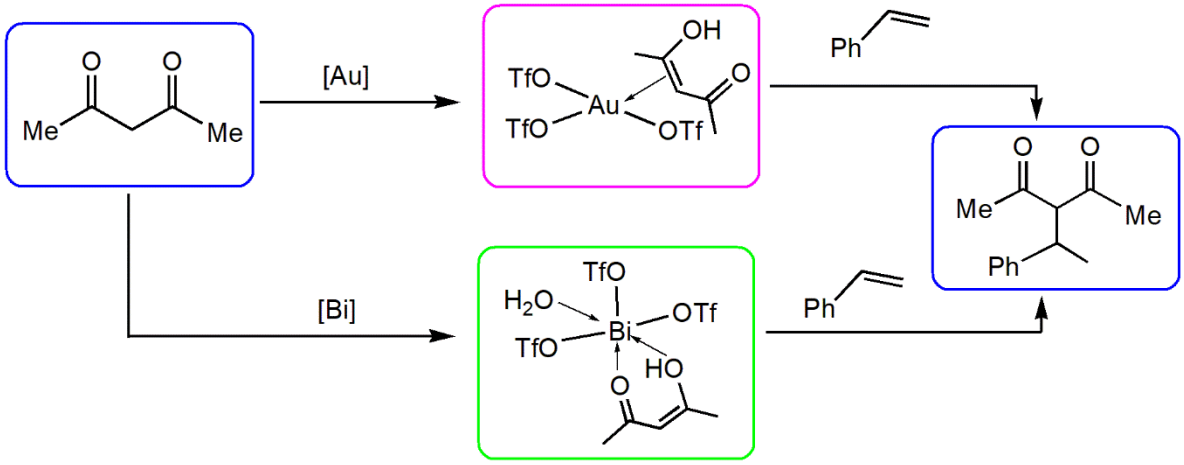
Density functional theory (DFT) has been used to investigate the mechanism of the experimentally efficient hydroalkylation of styrene with acetylacetone in the presence of a bismuth catalyst. It is shown that the mechanism is fundamentally different to that of the analogous gold-catalysed reaction, even though it leads to the same product. Our predicted mechanism allows good agreement to be obtained with all the experimental data.



Same product, different mechanisms