Theoretical Rationale for Regioselection in Phosphine Catalyzed Allenoate Additions to Acrylates, Imines and Aldehydes

Travis Dudding* and Evan Mercier
Department of Chemistry Brock University, St Catharines ON, Canada

A rationale for regioselection in phosphine promoted annulations of acrylates, imines and aldehydes with allenoates has been developed using computation at the B3LYP/6-31G(d) level of theory. The computed transition states revealed that Lewis acid activation, strong hydrogen bonding (H-bonding) and minimization of unfavorable van der Waals contacts are the guiding factors responsible for regioselection. An excellent level of correlation between the calculated regioselectivities and experiment was observed.