Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

On Ligand-free Palladium Cluster Catalysed Suzuki-Miyaura Reaction

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Supporting Information

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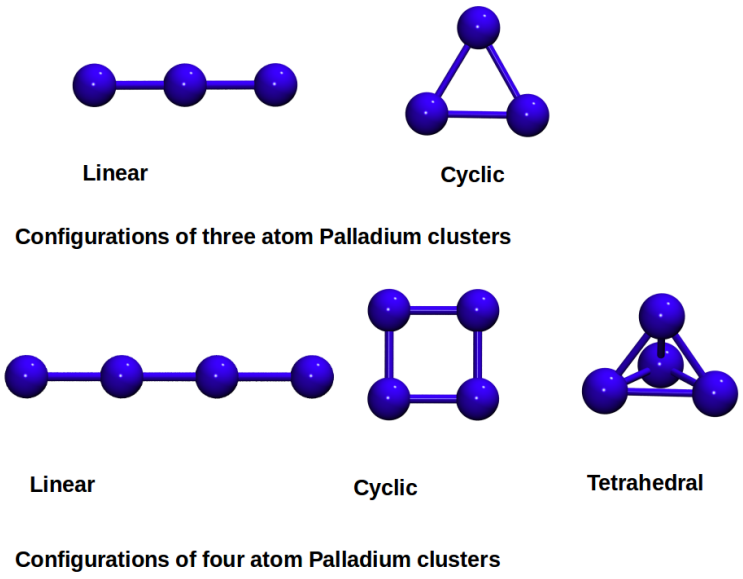

Figure S1: Different configurations for three- and four-atom palladium clusters

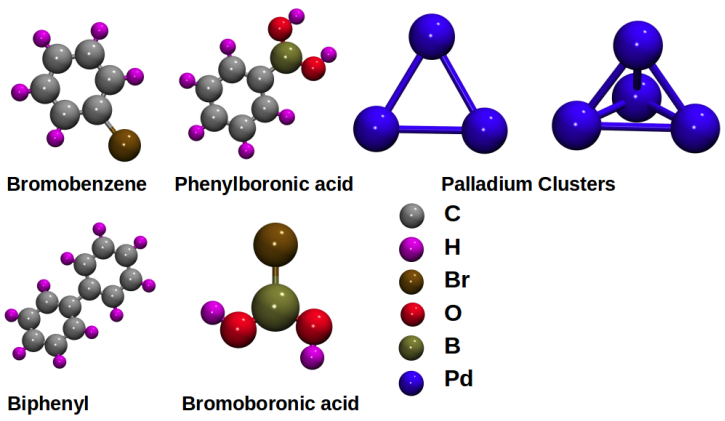

Figure S2: DFT optimised structures of reactants, products and catalysts reported in this study

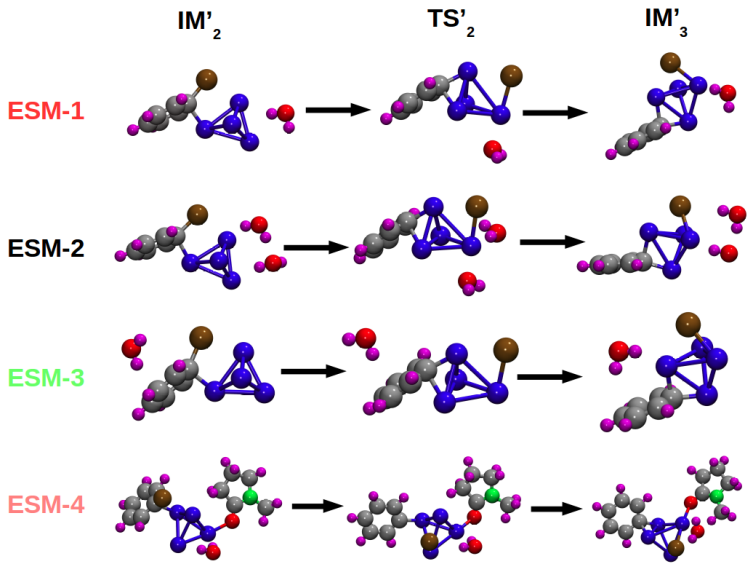

Figure S3: DFT optimised structures of rate limiting oxidative addition complexes over Pd_4 cluster in the presence of explicit solvents, water and N-Methyl-2-pyrrolidone

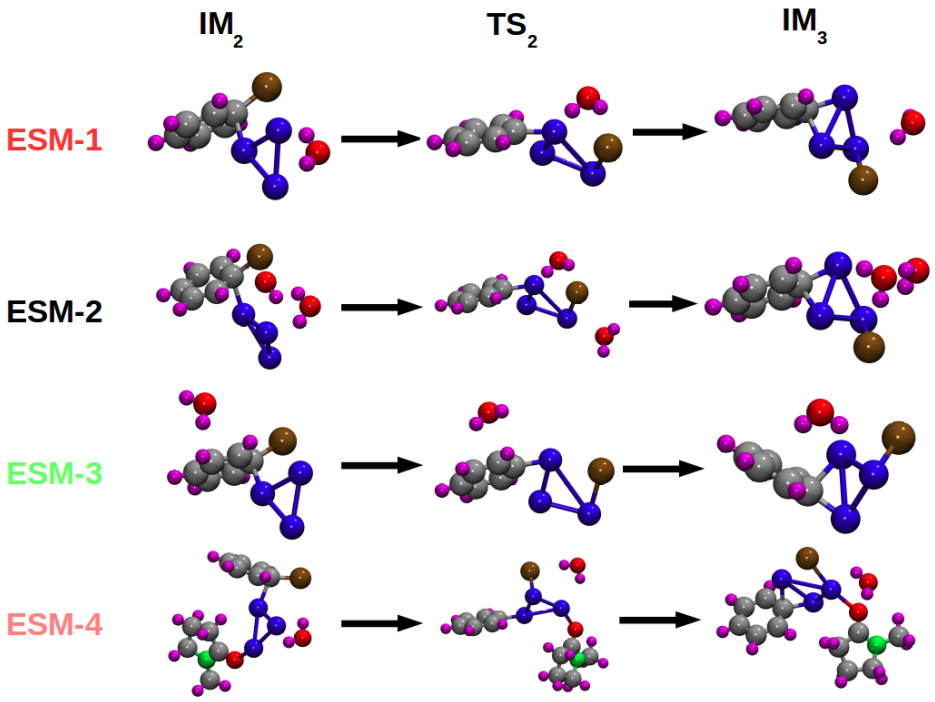

Figure S4: DFT optimised structures of rate limiting oxidative addition complexes over Pd_3 cluster in the presence of explicit solvents, water and N-Methyl-2-pyrrolidone

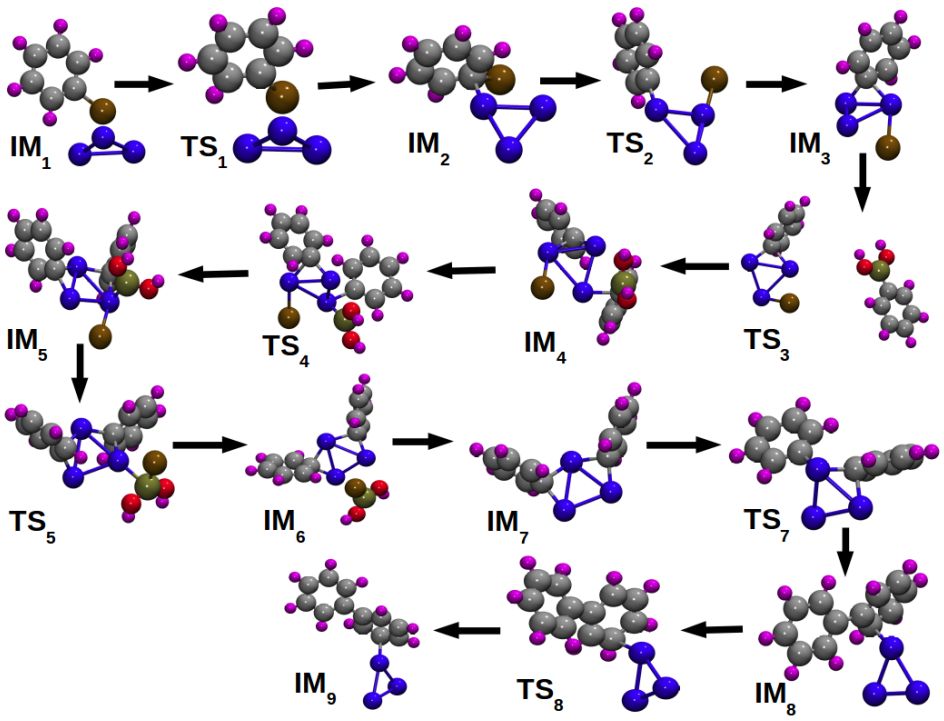

Figure S5: DFT optimised structures of transmetalation complexes over Pd_3 cluster

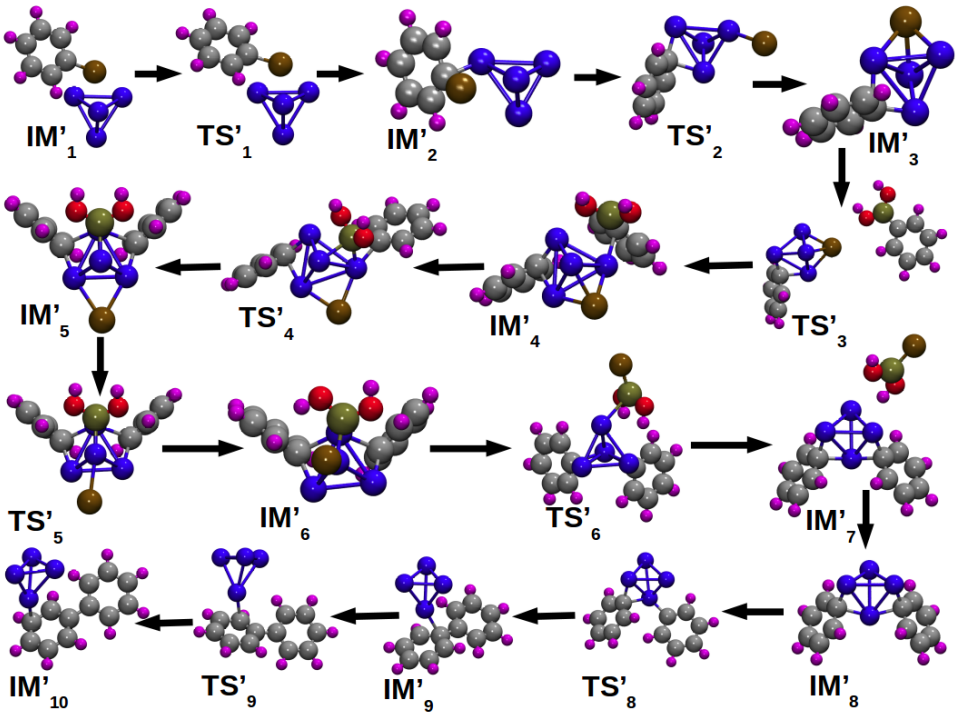

Figure S6: DFT optimised structures of transmetalation complexes over Pd_4 cluster

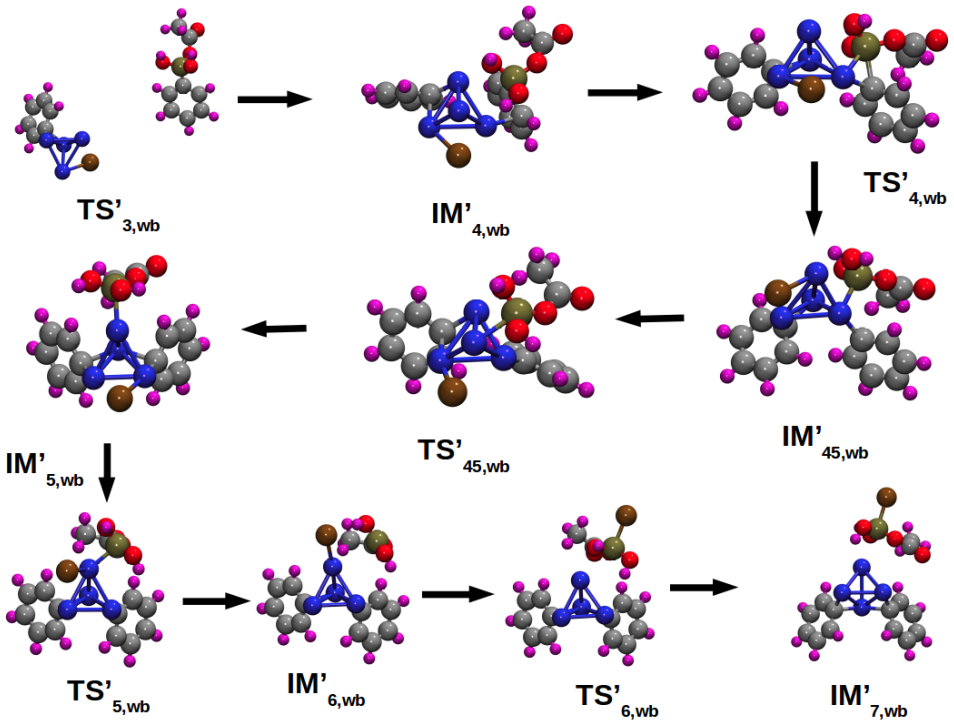

Figure S7: DFT optimised structures of transmetalation complexes over Pd_4 cluster in the presence of CH_3COOK

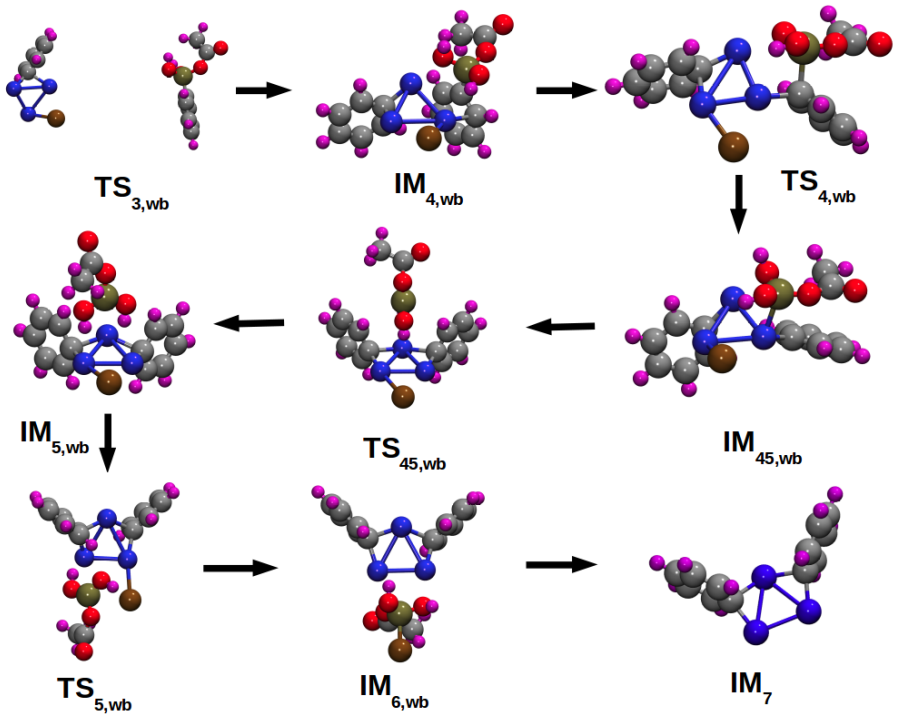

Figure S8: DFT optimised structures of transmetalation complexes over Pd_3 cluster in the presence of CH_3COOK