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Theoretical Insight into Ligand Free Manganese Catalyzed C-O Coupling Protocol for the Synthesis of Biaryl Ethers

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Abstract : Ullmann coupling reactions are gaining great relevance owing to their contribution in the synthesis of biologically and pharmaceutically important compounds. Palladium and many other heavy metals have proven their excellent ability in coupling reaction, but the toxicity matters. The first-row transition metal also possess toxicity, except in the case of iron and manganese. The suitability of manganese as a catalyst is achieving great interest in oxidation, reduction, C-H activation, coupling reaction etc. In this presentation, we discuss the thermo chemistry of ligand free manganese catalyzed C-O coupling reaction between phenol and aryl halide for the synthesis of biaryl ethers using Density functional theory techniques. The mechanism involves an oxidative addition-reductive elimination step. The transition state for both the step had been studied and confirmed using Intrinsic Reaction Coordinate (IRC) calculation. The barrier height for the reaction had also been calculated from the rate determining step. The possibility of other mechanistic way had also been studied. To achieve further insight into the mechanism, substrate having various functional groups is considered in our study to direct their effect on the feasibility of the reaction.

Keywords : Density functional theory, Molecular Modeling, ligand free, biaryl ethers, Ullmann coupling
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