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$C_{59}Pd$: A Heterogeneous Catalytic Material for Heck Coupling Reaction

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Abstract : Density functional theory calculations were carried out for identification of an active heterogeneous catalyst to carry out Heck coupling reaction which is of pharmaceutical importance. One of the carbonaceous nanomaterials, heterofullerene, was designed for the reaction. Stability and reactivity of the proposed heterofullerenes (C59M, M = Pd/Ni) were established with insights into the metal-carbon bond, electron affinity and chemical potential. Adsorbent potentials of both the heterofullerenes were examined from the adsorption study of four halobenzenes (C6H5F, C6H5Cl, C6H5Br and C6H5I). Oxidative addition activities of all four halobenzenes were investigated by developing free energy landscapes over both the heterofullerenes for rate determining step (oxidative addition). C6H5I showed a good catalytic activity for the rate determining step. Thus, C6H5I was proposed as a suitable halobenzene and complete free energy landscapes for Heck coupling reaction were developed over C59Pd and C59Ni. Smaller activation barriers observed over C59Pd in comparison with C59Ni put us in a position to propose C59Pd to be an efficient heterofullerene for carrying Heck coupling reaction.

Keywords : metal-substituted fullerene, density functional theory, electron affinity, oxidative addition, Heck coupling reaction
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