Quantum Chemistry Evaluation of the Mechanism of Catalyzed Alkylation of Indole Derivatives by Pd

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In this study, calculations of the formation of base metal methane in the presence of palladium acetate catalysts using the RB3LYP method were investigated computatively. In this study, triethyl amine used as a source of carbon and palladium used as an activating compound to break the bonds between carbon and hydrogen atoms (CSP3-H) The electron factors lead to the displacement in the position of 3 indole loops. The quenching of triethylamine leads to the formation of an intermediate palladium and it reacts by activating carbon-hydrogen bond. Finally, it makes a product called 1 and 1-base is an indoleyl methane, which is the result of substitution on the ring at position 3. In this reaction, by drawing a precise form for the minima and transition states, and determining and confirming the structure and energy of the points on the PES, and obtaining the activation energies in the desired reaction path, we have been looking for the determination of route and yield regions for triethylamine as carbon source and the curves of beginning and end points and transitional states. Keyword: Indol- Palladiumacetate- Alkylation- Tri-Amin - Triethylamine-C-H Aliphatic- B3LYP method

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