Detailed Quantum Studies on the *m*-Benzyne Diradical and the [3+2]cycloaddition Reaction Mechanism

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It is important to understand the nature of diradicals due to their potential roles in the formation of buckyballs and polymers and as intermediates in the combustion of polyaromatic hydrocarbons (PAHs). Buckyballs are currently explored for their potential usage in cancer treatment, and polyaromatic hydrocarbons are known for their damaging effects to the environment. Geometry optimizations of both the singlet and triplet states of meta-benzyne was performed using multi-reference methods(CAS(8,8), MCSCF, MR-CI, MR-AQCC) to characterize singlet-triplet gaps and radical electron coupling. Programs Gaussian and Columbus were used to obtain data. A separate study focused on analyzing the reaction mechanism of the pericyclic [3+2] cycloaddition between 1,1-cyclopropanediester and 1- methylindole. Two possible pathways, concerted and stepwise, were studied. Geometry optimization and frequency calculations were performed with the Gaussian program to determine the interaction between reactants, products, transition states, and intermediates.