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Computational Computation of the Efferene Structure on the Para phenylene diamine

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Abstract

In this study, the effect of fullerene electron mobility on the composition of paraphenylenediamine and stability was studied. Using quantum chemistry calculations, the first combination of paraffenylenediamine in a single-full-time region connected with fullerene through carbon atoms was reported. Experimental research was simulated and optimized using GIS software. Then the NBO calculations were performed on them. All calculations using the gossip software were performed in the 6-31 G * base series of the Factor Faster Phase. The results showed that when the compound is connected to the fullerene, the energy gap and its chemical hardness are low , Thus increasing its reactivity and bipolarity. Also, the natural gravity of volt-quantum capacities was considered comparing them in similar positions in compound interactions separately and fullerene. All evidence suggests that the electrons are fullerene and the transfer of electrons from paraffenylenediamine to fullerene.

Keywords: paraffenylenediamine, Fullerenes, Chemical potential.