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NATURAL BOND ORBITAL (NBO) POPULATION ANALYSIS OF $OS_3 (CO)_{10}\{M\text{-}PH_2PC (ME)_{2PPH2}\}$

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ABSTRACT

The molecular structure of $Os_3(CO)_{10}\{m\text{-}Ph_2PC(Me)_2PPh_2\}$ (1-me2) was calculated by the b3lyp density functional model using LANL2DZ basis set for os and 6-31g(p, d) for other atoms. Stability of the molecule arising from hyper conjugative interaction and charge delocalization has been analyzed using natural bond orbital (NBO) analysis. The second order perturbation energies of the most interaction NBOs and the population of electrons in core, valance and rydberg sub-shell have been predicted by density functional theory (DFT) computation Gaussian 09w software package. The natural atomic orbital occupancies showed the presence of charge delocalization within the molecule .the natural hybrid atomic orbital studies to Know about the type of orbital's and its percentage of s-type and p-type character.

KEYWORDS: Density Functional Theory Natural Atomic Orbital, Natural Bond Orbital