

Fascinating chemistry of mutually compatible symmetrical/ asymmetrical and bulky heterocyclic β -diketones-modified zirconocene dichloride: DFT assisted optimized molecular structure of $C_{33}H_{32}N_2O_4Zr$ containing two unequal Zr-Cp bonds

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Mutually compatible bulky heterocyclic β -diketones and symmetrical/ asymmetrical β -diketones- modified zirconocene dichloride products of the general formula $[Cp_2ZrLL']$ (where $LH = RCOC:C(OH)N(C_6H_5)N:CCH_3$ and $L'H = R'COCH_2COR''$, $R = -CH_3$ ($L_{(1)}H$), $R = -CH_2CH_3$ ($L_{(2)}H$), $R = -C_6H_5$ ($L_{(3)}H$), $R = p-CIC_6H_4-$ ($L_{(4)}H$) and $R' = R'' = -CH_3$ ($L'_{(1)}H$), $R' = -CH_3$, $R'' = -C_6H_5$ ($L'_{(2)}H$), $R' = R'' = -C_6H_5$ ($L'_{(3)}H$)) have been generated by the reactions of zirconocene dichloride with mutually compatible bulky heterocyclic β -diketones and symmetrical/ asymmetrical β -diketones in the presence of triethylamine in 1:1:1:2 molar ratio in refluxing dry THF. On the basis of spectroscopic and mass studies, tentative structures of these complexes have been suggested. Density functional theory (B3LYP) has been employed to study the optimized molecular structure, optimized energy, stability, distortions of optimized geometry and energy gap of one representative zirconocene complex to corroborate the structures of these complexes.

Keywords: Zirconocene complexes, β -Diketones, Unequal Zr-Cp bonds, Optimized energy, Optimized geometry