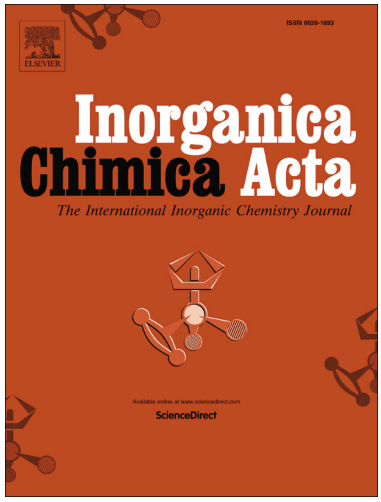

Research paper

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Impact of Functional Groups Substitution on the Molecular Properties of Magnesium and Scandium Phthalocyanines

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Abstract:

This investigation reports the molecular properties of magnesium and scandium phthalocyanines, substituted with different functional groups such as methyl (CH_3), hydroxyl (OH), amine (NH_2), carboxyl (COOH) and aldehyde (CHO) using DFT method. The structure reveals that substituted Mg-Pc possess planar configuration in which the Mg atom lies along the Pc plane while the substituted Sc-Pc acquires shuttlecock structure where Sc protrudes out of the Pc plane. Substituted Mg-Pcs are more stable when compared to substituted Sc-Pcs and functionalization plays an important role in enhancing the molecular properties of M-Pcs. Substitution of amine, hydroxyl and methyl groups renders electron donating character while the carboxyl and aldehyde substitutions make M-Pcs electron acceptors, respectively. The HOMO-LUMO gap character in substituted M-Pcs implies their utilization in the area of organic solar cells and gas capturing applications.

Keywords: functional groups, magnesium, scandium, phthalocyanine, reactivity parameters

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