

Study of the molecular properties of mono- and binuclear metal s-indacenyl complexes with Ir, Rh, and Re: A theoretical approach

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Density functional theory (DFT) calculations were performed on a new family of mono- and bimetallic complexes, containing 4,8-([10]paracyclophane)-1,5-dihydro-s-indacene as the bridging ligand between the two metallic centers and different ancillary ligands. The s-indacene was blocked by substitution of the central benzene ring with the [10]paracyclophane to obtain the syn-conformations. This would force the metallic centers to be close together. It is proposed, due to the calculated molecular and electronic properties such as the reactivity indexes, the delocalized nature of the s-indacenyl ligand, and the electron-rich metals, that these systems could be reactive in a catalytic reaction. The results indicate that the systems with Rh and Re holding ancillary ligands such as bipy and CO show the best properties to be active in a chemical reaction. In this sense, by the assessed geometrical and electronic properties, when compared with a previously reported system, these complexes could be candidates for the reduction of CO₂ to oxalate. © 2017 Ximena Zarate et al.