Theoretical Evaluation of Electron Delocalization in Organometallic Compounds: From Agostic Bond to Aromaticity

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Abstract. Electron delocalization plays a key role in several fundamental phenomena present in organometallic chemistry such as chemical bond and aromaticity.[1] Organometallic compounds show a wide variety of interactions which have no counterpart in purely organic molecules. Some of the most significant interactions are the agostic and hydrogen bonds. In some cases the characterization of these interactions can cause controversy and the frontier between agostic and hydrogen bond becomes not clear. In the first part of this work, we propose a new tool to analyze the agostic bond by means of electron delocalization measures in the framework of the quantum theory of atoms and molecules (QTAIM).[2] Moreover, in organometallic compounds, aromatic organic ligands are commonly coordinated to transition metals and this complexation leads to a change on the aromaticity of the free ring. In certain cases, aromaticity decreases after coordination whereas sometimes the ligand becomes more aromatic. Here, we have analyzed the aromaticity of benzene ring in $(\eta^6\text{-}C_6H_6)Cr(CO)_3$ complex[3] and how the aromaticity of the porphyrin ligand is influenced by the nature of the central metal in metalloporphyrins.[4]

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