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QTAIM View of Metal-Metal Bonding in Trinuclear Mixed-Metal Bridged Ligand Clusters Containing Ruthenium and Osmium

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Abstract : Through DFT/QTAIM calculations, we have provided new insights into the nature of the M-M, M-H, M-O, and M-C bonds of the (Cp*Ru)n(Cp*Os)3−n(μ3-O)2(μ-H)(Cp* = η5-C5Me5, n= 3,2,1,0). The topological analysis of the electron density reveals important details of the chemical bonding interactions in the clusters. Calculations confirm the absence of bond critical points (BCP) and the corresponding bond paths (BP) between Ru-Ru, Ru-Os, and Os-Os. The position of bridging hydrides and Oxo atoms coordinated to Ru-Ru, Ru-Os, and Os-Os determines the distribution of the electron densities and which strongly affects the formation of the bonds between these transition metal atoms. On the other hand, the results confirm that the four clusters contain a 6c–12e and 4c–2e bonding interaction delocalized over M3(μ-H)(μ-O)2 and M3(μ-H), respectively, as revealed by the non-negligible delocalization indexes calculations. The small values for electron density ρ(b) above zero, together with the small values, again above zero, for laplacian ∇2ρ(b) and the small negative values for total energy density H(b) are shown by the Ru-H, Os-H, Ru-O, and Os-O bonds in the four clusters are typical of open shell interactions. Also, the topological data for the bonds between Ru and Os atoms with the C atoms of the pentamethylcyclopentadienyl (Cp*) ring ligands are basically similar and show properties very consistent with open shell interactions in the QTAIM classification.

Keywords : metal-metal and metal-ligand interactions, organometallic complexes, topological analysis, DFT and QTAIM analyses

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