

Charge Density Studies on Heterobimetallic Phosphido-Bridged Mo and W Complexes

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The heterobimetallic phosphido-bridged complexes, $\text{CpW}(\text{CO})_2(\mu\text{-PPh}_2)\text{Mo}(\text{CO})_5$ (**1**) with W-Mo distance 3.1723(4) Å and $\text{CpW}(\text{CO})_3(\mu\text{-PPh}_2)\text{Mo}(\text{CO})_5$ (**2**) with W-Mo distance 4.510(4) Å have been reported with special chemical reaction properties because of the interaction between W and Mo. For example, complex **2** will be converted into **1** after irradiation with UV or heating at reflux temperature. In order to realize how chemical bonds influence the reaction properties in complex **1** and **2**, the X-ray diffraction data of both complexes at 100 K are collected and the experimental electron density in terms of multipole model are used to investigate the electron density distribution and chemical bonds. All chemical bonds will be quantified based on atoms in molecule (AIM) theory to elucidate the nature of those interactions. All interactions are verified by the location of the bond critical point and its associated topological properties, such as local density, Laplacian, and energy density at bond critical points. Moreover, the isovalue surface of Laplacian charge density distribution and the detailed atomic graph around each atomic site will reveal the shape of the valence-shell charge concentration and provide a reasonable interpretation of the bonding in each atom. All extracted chemical bonding characters from experimental charge density will be further compared with the density functional theory calculation and give out a reasonable explanation related to the different chemical reaction properties between **1** and **2**.