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Molecular Electrostatic Potential and Electron Density Topography: Structure and Reactivity of (substituted arene)$Cr(CO)_3$ Complexes

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Structural properties as well as subtle electronic effects occurring in (substituted arene)-$Cr(CO)_3$ complexes have been investigated at HF, B3LYP, and MP2 levels using the topographical properties of the molecular electrostatic potential (MESP) as well as electron density. The most stable structures are characterized as syn-eclipsed for an electron-donating arene substituent and anti-eclipsed for an electron-withdrawing arene substituent. The MESP topography unambiguously revealed the electronic nature of the $Cr(CO)_3$ moiety as a very strong electron-withdrawing group to the arene unit of the complex. Interestingly, the substituent effects are strongly felt at the MESP surrounding the carbonyl oxygen rather than the arene ring. The effect of electron correlation significantly changes the values of the MESP at CPs, especially in the case of systems with an electron-withdrawing substituent. The electron density topography revealed that only the three ring carbon atoms that are syn with respect to the carbonyl groups are bonded to the chromium atom via a (3, −1) bond critical point, suggesting a trigonal-prismatic structure for these complexes.