

Near-Edge X-ray Absorption Fine Structure spectroscopy study of organometallic sandwich compounds and functionalized polymers.

Edwige Otero and Stephen G. Urquhart

Department of Chemistry, University of Saskatchewan, Saskatoon, SK, S7N 5C9, Canada.

Ferrocene and metal arene functionalized materials are finding a wide application in polymeric, molecular electronics and bioorganometallic materials. The interpretation of the NEXAFS spectra of organometallic compounds is difficult due to the complexity of the interactions between the metal and its surroundings. Two approaches are commonly used, an atomic multiplet model and covalent bonding model, leading to conflicting spectral assignments. To determine which of the models is most appropriate for the study of metallocene and metal arene, we have recorded NEXAFS spectra of series of substituted ferrocenes and substituted (η^6 -benzene)(η^5 -cyclopentadienyl)iron(II) hexafluorophosphate compounds. With the aid of density functional theory and extended Hückel molecular orbital theory calculations we have interpreted these spectra. Our results indicate that the covalent bonding model is the most appropriate for closed shell molecules ($3d^6$, low spin), but is less effective for open shell molecules ($3d^5$, low spin). These findings help us to characterize the spectra of metal arene compounds and functionalized polymers.