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Application of photoelectron spectroscopy to study electronic ligand effects on iron cyclopentadienone complexes

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Organometallic chemistry is a key process in homogenous catalysis and gives access to a wide range of products and reactions. Through their steric and electronic effects, ligands are able to orientate the reactivity of the complexes and can thus influence the selectivity in the chemical transformations. Usually, the metal-ligand bond is depicted by the Dewar-Chat-Duncanson model^{1,2} involving two opposite interactions, a σ -donor and a π -acceptor effect. Over the years, many experimental methods have been developed to measure these electronic effects, the most common being that of Tolman (Tolman electronic parameter), which is limited to organometallic complexes possessing probe ligands such as CO and based on the A₁-symmetrical CO-stretching frequency shift.³

We have recently developed the use of new experimental gas-phase approaches to measure these effects, one based on photoelectron spectroscopy (PES) coupled to synchrotron radiation, and the other on mass spectrometry using activation by higher energy collision dissociation (HCD). Under the first method, the satisfying results obtained on model systems⁴ have encouraged us to apply this method to catalysts developed for hydrogenation reactions,⁵ and to probe the electronic interaction between the ligand and the metal centre. Results obtained for tricarbonyl iron complexes of the $(\text{Fe}(\text{CO})_3\text{L})$ type, with L being substituted cyclopentadiene ligands, are presented here. The photoelectron spectra provide access to the ionization energies and state-selected Fe-CO dissociation energies.

References

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