High-spin Cyclopentadienyl Complexes, Part 7.
Ambivalent Interpretation of the Bonding in Iron-Copper Complexes:
Metalated Arene versus Carbocyclic Carbene

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\textit{Dedicated to Professor Otto J. Scherer on the occasion of his 75\textsuperscript{th} birthday}

The electron distribution within a mesityl ligand bridging a cyclopentadienyliron fragment attached to the mesityl $\pi$ system and a second metal fragment connected to the ipso carbon of the mesityl ring has been probed using a copper(I) halide as a component in $[\text{Cp}''\text{Fe}(\mu,\eta^5:\eta^1-C_6H_2Me_3)\text{CuCl}]$ (2) and its copper bromide derivative 3. This approach minimizes steric effects and allows for DFT calculations the results of which are in very good agreement with structural data. The calculations show a significant carbene character already for the bare phenyl anion as a result of electrostatic repulsion of the lone pair pushing the $\pi$ electrons away from the ipso carbon towards the para carbon atom of the aromatic ring. $\pi$ Coordination of a cyclopentadienyliron(II) fragment to the phenyl anion to form a hypothetical sandwich complex does not change this situation. The iron center rather follows the unsymmetric distribution of $\pi$ charge with an unsymmetrical coordination to the $\pi$ system. Coordination of a copper(I) chloride moiety to the phenyl anion or to the hypothetical $\pi$ complex $[\text{CpFe}(C_6H_3)]$ in both cases equally lowers that carbene character by attracting the lone pair of the ipso carbon and thus decreasing its repulsive influence on the $\pi$ electrons.

\textit{Key words:} Iron Complexes, Copper Complexes, Tri(tert-butyl)cyclopentadienyl, DFT Calculations, Carbene