

Reading instructions for “Designing Molecules for Metal–Metal Electronic Communication: Synthesis and Molecular Structure of the Couple of Heterobimetallic Isomers $[\eta^6\text{-}(2\text{-Ferrocenyl})\text{indene}]\text{-Cr}(\text{CO})_3$ and $[\eta^6\text{-}(3\text{-Ferrocenyl})\text{indene}]\text{-Cr}(\text{CO})_3$

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Things to think about while reading:

- Are you convinced by the authors’ explanation of why **1** adopts a planar Cp-indenyl conformation while **2** does not? Are there any factors that seem to be missing from their analysis?
- The authors make a lot of inferences about these molecules based on carbonyl stretching frequencies, which we are also familiar with. How does the proposed π -hydrogen bond in complex **1** account for the lowered IR frequencies and splitting of the tricarbonyl E band at low temperature? How can we rationalize the relationship between internuclear charge transfer and the carbonyl IR shifts on oxidation?
- How is the DFT fragment analysis consistent with and/or problematic for the electronic coupling inferred from CV and IR results?

Background/definitions:

- Heterobimetallic: describes a complex containing two metal centers of different identities.
- Cyclic voltammetry: a technique that measures current as a function of an applied voltage. It can therefore be used to determine oxidation and reduction potentials.
- Intervalence charge transfer (IVCT): a process that transfers an electron between adjacent metallic sites whose oxidation states are unequal.
 - $L_xM^{p+}\text{-}[\text{bridge}]\text{-}M^{q+}L_y + h\nu \rightarrow L_xM^{(p+1)+}\text{-}[\text{bridge}]\text{-}M^{(q-1)+}L_y$