



## Can Polynuclear Metal Clusters Behave as "Extended" Organometallic Complexes?

Nielsen, Martin; Betley, Theodore A.

*Published in:*  
Book of Abstracts, Sustain 2017

*Publication date:*  
2017

*Document Version*  
Publisher's PDF, also known as Version of record

[Link back to DTU Orbit](#)

*Citation (APA):*  
Nielsen, M., & Betley, T. A. (2017). Can Polynuclear Metal Clusters Behave as "Extended" Organometallic Complexes? In *Book of Abstracts, Sustain 2017* Article E-16 Technical University of Denmark.

---

### General rights

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

## Can Polynuclear Metal Clusters Behave as "Extended" Organometallic Complexes?

Martin Nielsen<sup>1,2</sup> and Theodore A. Betley<sup>2</sup>

<sup>1</sup> DTU Chemistry, Technical University of Denmark

<sup>2</sup> Department of Chemistry and Chemical Biology, Harvard University

In the past few years, our group has demonstrated the synthesis of the hexanuclear iron cluster (HL)<sub>2</sub>Fe<sub>6</sub> and its redox potential, which spans at least 7 redox steps. The hexanuclear core comprises an octahedral structure with an iron metal positioned on each of the six vertices, each possessing one vacant coordination site directed outwards from the center of the Fe<sub>6</sub> octahedral. The cluster HOMO is a triply degenerate orbital of t<sub>1u</sub> symmetry, approximating three p-orbitals equally distributed over two iron centres *trans* to each other. This set up the possibility to perform chemistry on the cluster much alike what we know from classic organometallic chemistry, and a range of questions needs to be addressed: Does the cluster undergo oxidative addition and would it be *trans* and/or *cis* selective? What is the mechanism? In principle, up to three consecutive oxidative additions are possible; can we control that? Is the reverse, reductive elimination, feasible? Are there *cis/trans* effects over the core such that e.g. an iron centre would be influenced by the ligation of its *trans* iron partner?

We strive to answer these questions, and our findings this far will be presented.