Homogeneous reduction by bifunctional manganese catalysis
a quantum chemical approach

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Propositions

accompanying the dissertation

Homogeneous reduction by bifunctional manganese catalysis: a quantum chemical approach

by

Annika Meike Krieger

1. Machine learning will only be successfully applied in identifying novel active catalytic species if research groups start regularly reporting inactive and mediocre catalytic systems.
2. Rate-determining or enantio-determining steps must be theoretical explained by a kinetic model that accompanies DFT calculations (Chapter 5).
3. Explaining outliers is more significant than observing trends.
4. The conditions under which a catalyst operates are just as important as its structural properties (Chapter 3).
5. Questioning state-of-the-art methodology is important for scientific progress (Chapter 6).
6. Financing research projects at university with funds from (multinational) companies endangers the independence of the research.
7. The term "sustainable" is not well-defined, leading to an overuse in scientific publications.
8. It is not desirable to implement manganese in industrial catalysts because it stimulates social injustice and environmental degradation.[1]
9. High-throughput calculations can only be meaningful if they can be related to experimental data.
10. Gender quotas must be implemented at all levels of an organisation to successfully reach diverse executive boards.

These propositions are regarded as opposable and defendable, and have been approved as such by the promotors prof. dr. E.A. Pidko and dr. G. Li.

[1] A. González, J. Wilde-Ramsing, P. Ngoatje, N. Soekoe, F. Vally, S. Kwizera and S. Dladla, *Manganese Matters: A metal of consequence for women and communities in South Africa affected by mining and the global energy transition*, ActionAid Netherlands (2021).