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## Reactivity of cobalt(II)-dichalcogenide complexes: correlation between redox conversion and ligand-field strength

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# Propositions (Stellingen)

accompanying the thesis

## Reactivity of Cobalt(II)-Dichalcogenide Complexes: Correlation between Redox Conversion and Ligand-Field Strength

1. Estimation of *d*-orbital splitting energy of transition metal compounds can be obtained *in silico*.

*This thesis Chapters 2, 3, and 4.*

2. Formation of side products often leads to a greater understanding of the reaction.

*This thesis Chapter 2 and Chapter 3.*

3. A rational design of disulfide ligands for the redox-conversion reaction of Co(II)-disulfide to Co(III)-thiolate complexes is paramount.

*S. Itoh, et al., JACS, 2001, 123, 17, 4087-4088; Y. Ueno, et al., JACS, 2002, 124, 42, 12428-12429; E.C.M. Ordning-Wenker, et al., Inorg. Chem, 2014, 53, 16, 8494-8504; This thesis Chapter 5.*

4. The magnitude of the overall *d*-orbital splitting energy of a complex controls the cleanliness of its redox-conversion reaction for the Co(II)/Co(III) system.

*This thesis Chapter 2, 3, 4, and 5.*

5. It is important for new types of reaction to use consistent terminology.

*H. Jeong, et al., RSC Adv., 2019, 9, 9049; E.C. Constable, et al., Dalton Trans., 2008, 3795-3797; J-A. Yan, et al., Inorg Chem., 2017, 56, 9055-9063. A.M. Thomas, et al., JACS, 2013, 135, 18912-18919; Y. Ueno, et al., JACS, 2002, 124, 42, 12428-12429; E.C.M. Ordning-Wenker, et al., Inorg. Chem, 2014, 53, 16, 8494-8504;*

6. Conclusions regarding the reversibility of Co(II)-disulfide to Co(III)-thiolate conversion cannot be drawn based on the Cu(I)-disulfide to Cu(II)-thiolate conversion.

*M. Gennari, et al., Angew. Chem. Int. Ed., 2014, 53, 5318-5321*

7. Estimation of the *d*-orbital splitting energy in a lower symmetry system should be based on the difference between energy of the highest and the lowest-lying molecular orbitals with largest *d*-orbital contribution.

*T. Ishii, et al., Dalton Trans., 2009, 680-687; V.G. Chilkuri, et al., Inorg Chem., 2020, 59, 984-995*

8. Scientific publications should not only describe the positive results.
9. Systematic screening of crystallization conditions is preferred over blind attempts to grow single crystals.
10. Doing research requires the willingness to embrace failures and learn from mistakes.
11. Lack of resources inspires creativity.

Christian Marvelous

*Leiden, July 2022*