

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.*
- 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. Ording-Wenker, et al., Inorg. Chem, 2014, 53, 16, 8494-8504; This thesis Chapter 5.
- 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.*
- 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. Ording-Wenker, et al., Inorg. Chem, 2014, 53, 16, 8494-8504;
- 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

- 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

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