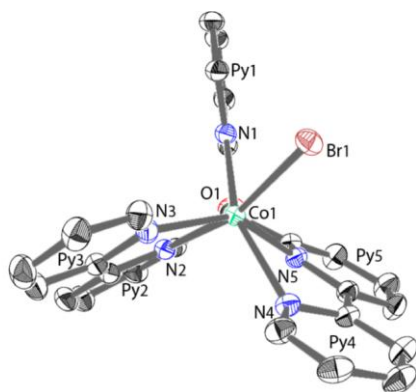


Synthesis and Activity of Substituted Cobalt Polypyridyl Water-Reduction Catalysts.

Peter Müller¹, Roger Alberto¹

¹University of Zürich Department of Chemistry, Winterthurerstr. 190, CH-8057 Zürich, Switzerland

E-mail: Peter.mueller@chem.uzh.ch Today, more than 80% of the global energy supply is covered by fossil fuels. Beside the fact that these energy sources are not renewable, their use also causes several environmental Problems.^[1] Therefore, the replacement of fossil fuels by renewable energy sources has main importance.



Our group showed already promising results in water reduction with different cobalt polypyridyl catalysts.^[2] One of the most promising catalysts, the so-called Co-apenta was selected for further studies. As the crystal structure of **1** shows (Fig. 1), the nitrogen atom of one of the bipyridyl subunits and the bromide occupy the axial positions of the polyhedron.

Fig. 1. Crystal structure of Co-apenta. The complex shows a strongly distorted octahedral structure.^[2]

The position of the bromide leads to the conclusion, that protonation of the cobalt center takes place on this axial position. Therefore, different substituents in the *o*-position of the pyridine ring (Fig. 2) can help to prove this conclusion.

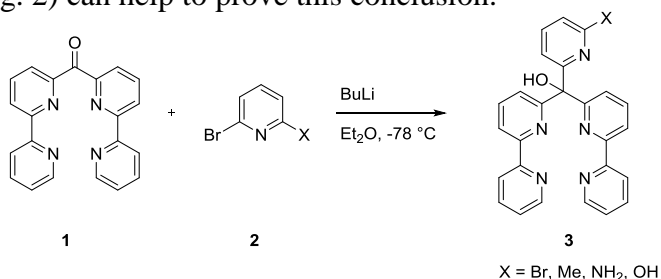


Fig. 2. Synthesis of the substituted polypyridyl ligands. For reasons of simplification, only the ligand system is drawn.

Steric substituents like methyl should lower the activity of the catalyst, whereas polar groups with the ability to form hydrogen bonds like amines or hydroxy groups should enhance the activity.

Funding: Swiss National Science Foundation (CRSII2 160801)

Acknowledgement: We thank the whole Alberto group for their support and especially the Swiss Nation Science Foundation for funding us.

References:

- [1] S. Styring, *Faraday Discuss.* **2012**, *155*, 357-376.
- [2] C. Bachmann, M. Gutentag, B. Spingler, R. Alberto, *Inorg. Chem.*, **2013**, *52*, 6055–6061.