A HYDROGEN BATTERY: REVERSIBLE HYDROGEN STORAGE IN THE CO_2/FORMIC ACID SYSTEM

Scope: The steady increase of renewable energy sources require an adaption of the current power grids. The problem is linked to the fluctuating nature of such energy sources which are driven by wind or sun power. Energy can no longer be generated on demand but must be harvested and stored when available. Therefore the need to reversibly store huge amounts of energy in a cheap, sustainable, and robust fashion has become a major challenge of our time.

Approach: The solution we propose can effectively deal with two mature issues of modern industry: Energy production releases vast amounts of carbon dioxide into the earth's atmosphere, contributing to global warming. Another problem is to store produced energy reversibly. However, electrolysis of water is a simple technique to transform electricity into chemical energy (H_2). The storage of large volumes of hydrogen gas is difficult, costly and lossy. In our approach, we combine hydrogen and CO_2 to obtain formic acid (FA). FA offers many advantages over the reactants such as storage at RT, moderate toxicity and not flammable below 85% in aqueous solution.

Chemistry: It is known that many transition metal complexes exhibit catalytic activity towards these reactions. The challenge is to find a set of ligands which is labile enough to allow the reaction to occur but at the same time protects the central ion against reduction by hydrogen. Promising results were achieved with combinations of phosphine containing ligands and ruthenium[1], as well as combinations of Cp*, bidentate nitrogen donor ligands and iridium.[2] An extremely durable catalyst is $Ru(TPPTS)_2Cl$, which properties will be further explored in this TP.

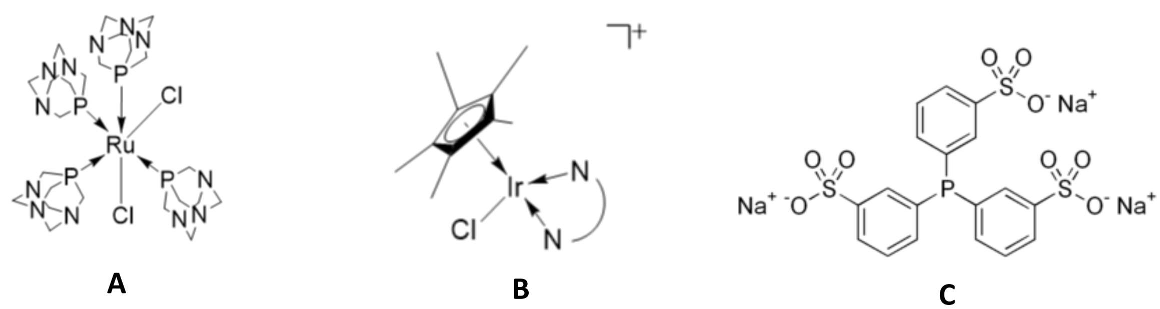

Figure 1 (A) $[Ru(PTA)_4Cl_2]$ reached an unprecedented high FA concentration in water without any additives (B) structure of precatalysts which exhibit good catalytic activity but show limited stability under harsh reaction conditions (C) structure of TPPTS

Methods: Microwave synthesis offers a fast and convenient way to synthesize plenty chemical compounds, a method which has huge future potential.[4] Another essential technique of this project will be multinuclear (^{1}H, ^{13}C, or ^{31}P) NMR spectroscopy in medium pressure sapphire tubes (up to 100 bar), enabling us to observe chemical reactions in real-time on a molecular level.

[1] S. Moret, P.J. Dyson, G. Laurenczy, Nature Communications **2014**, 5.
[2] C. Fink, G. Laurenczy, Dalton Transactions **2017**, 46, 1670-1676.
[3] M. Montandon-Clerc, A.F. Dalebrook, G. Laurenczy, J Catal **2015**.
[4] J. Tönnemann, J. Risse, Z. Grote, R. Scopelliti, Eur J Inorg Chem **2013**, 2013, 4558-4562.