Spectroscopic Study of Cr(III) in Water and Deep-Eutectic Solvents Using MCR-ALS

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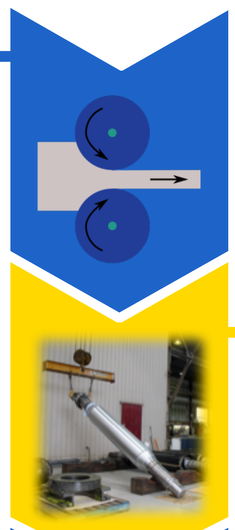
Introduction

Steel Production

During the cold rolling of steel, the thickness of the steel strips is reduced by applying a high pressure with two rolling cylinders.



Hard Chrome

These cylinders have to be protected from the harsh conditions. Hence, they are coated with a **hard chromium layer**.

Chromium(VI)

This layer is typically electro-deposited from an aqueous solution containing the toxic and carcinogenic Cr(VI).

Chromium(III)

Powered by the quest to a more **sustainable** production process, **OCAS NV** has already been working for six years on a patented Cr(VI)-free alternative, using a Cr(III)-based deep-eutectic solvent (DES) as electrolyte[1]. However, there still exists a lack of fundamental knowledge on the deposition mechanism.

Research Goal

This project focuses on the elucidation of the **coordination chemistry of the Cr(III) species** in the DES as a function of composition and the presence of additives to predict the in-use properties of the eventual hard chromium layer.

Methods

Samples

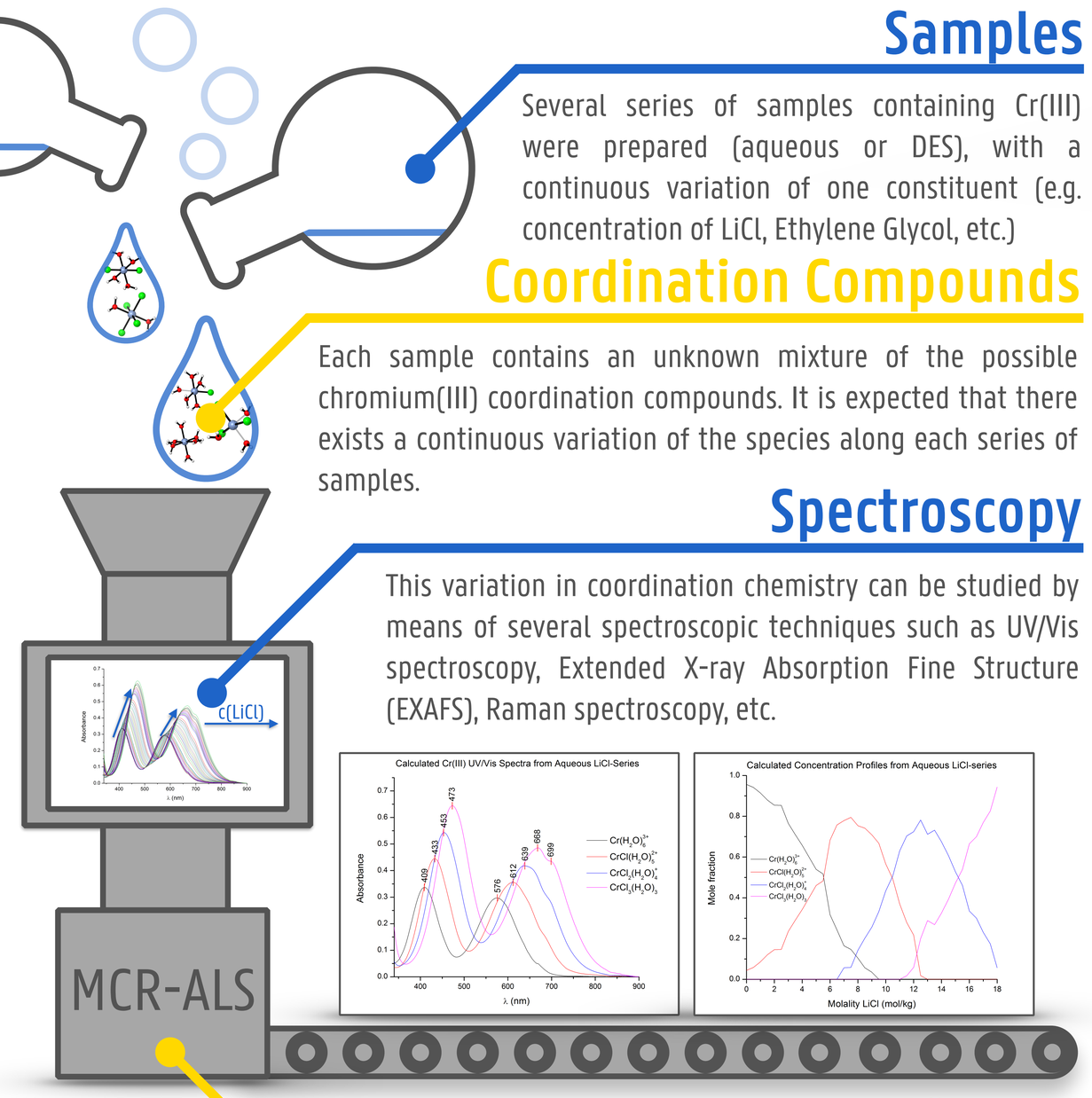
Several series of samples containing Cr(III) were prepared (aqueous or DES), with a continuous variation of one constituent (e.g. concentration of LiCl, Ethylene Glycol, etc.)

Coordination Compounds

Each sample contains an unknown mixture of the possible chromium(III) coordination compounds. It is expected that there exists a continuous variation of the species along each series of samples.

Spectroscopy

This variation in coordination chemistry can be studied by means of several spectroscopic techniques such as UV/Vis spectroscopy, Extended X-ray Absorption Fine Structure (EXAFS), Raman spectroscopy, etc.



MCR-ALS

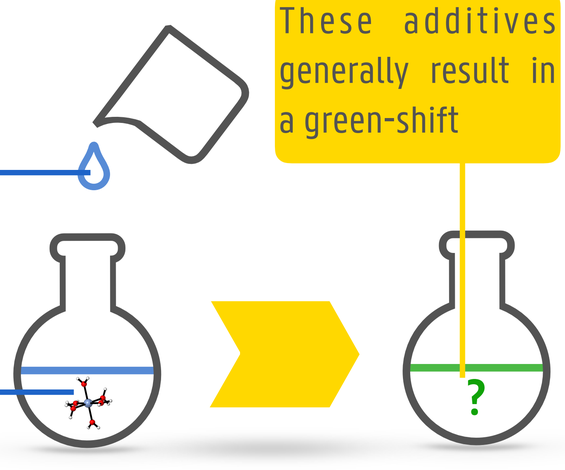
Multi-variate Curve Resolution - Alternating Least Squares (MCR-ALS)[2] is a chemometrical technique based on similar principles as Principal Component Analysis (PCA), but specifically designed for the deconvolution of series of spectra to the pure spectra of the constituents and the corresponding concentration profiles.

Sample Series

Possible additives:
- LiCl
- Ethylene Glycol + Choline Chloride
- Perchloric Acid
- Etc.

$CrCl_3.6H_2O$ dissolved in water results in hexaaquachromium(III) after equilibration (blue)

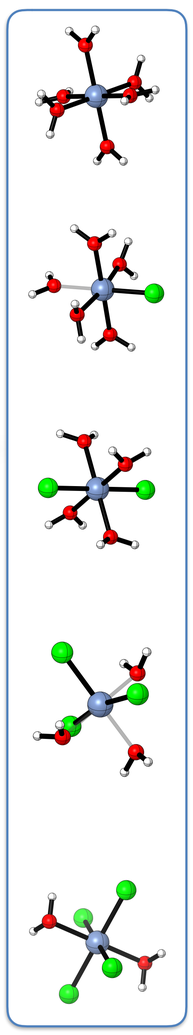
These additives generally result in a green-shift



Semi-industrial Pilot Line

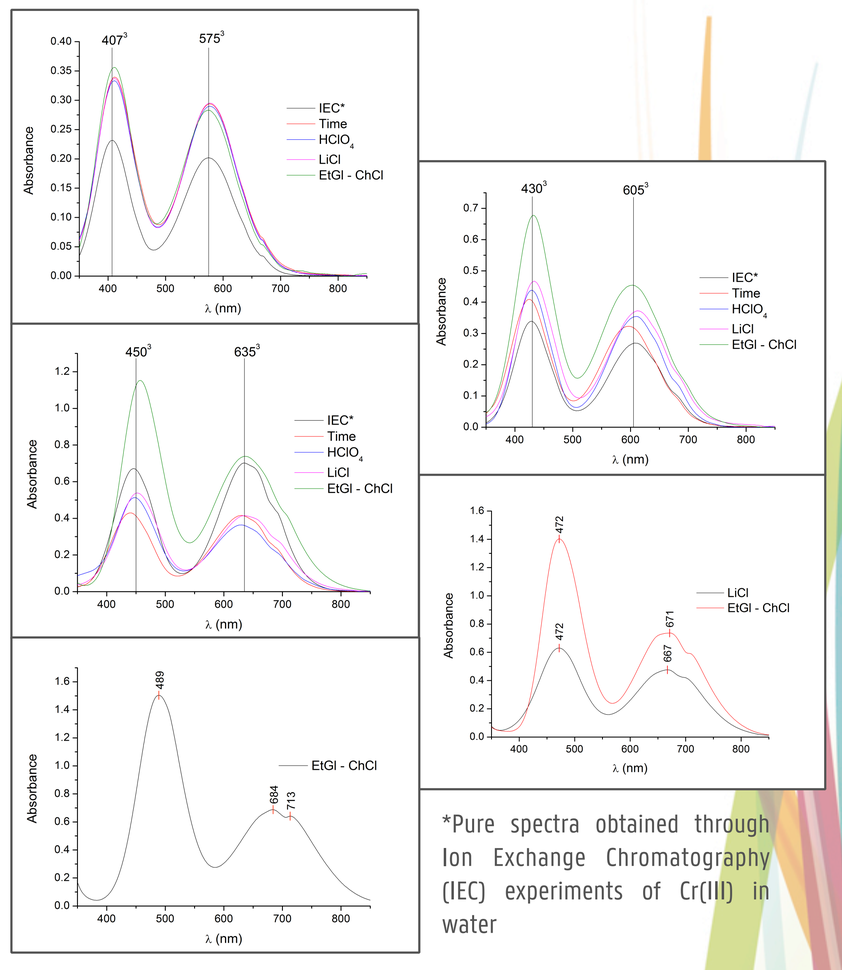
Due to the promising features of this new electrodeposition solvent, a flexible semi-industrial pilot plant has been designed in OCAS NV. In this way, several set-ups, IL compositions, additives, etc. can be tested and evaluated on a large scale, and compared with lab scale experiments.

Pure UV/Vis Spectra



Higher chlorinated chromium(III) species

Green-shift in UV/Vis spectra



*Pure spectra obtained through Ion Exchange Chromatography (IEC) experiments of Cr(III) in water

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References

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