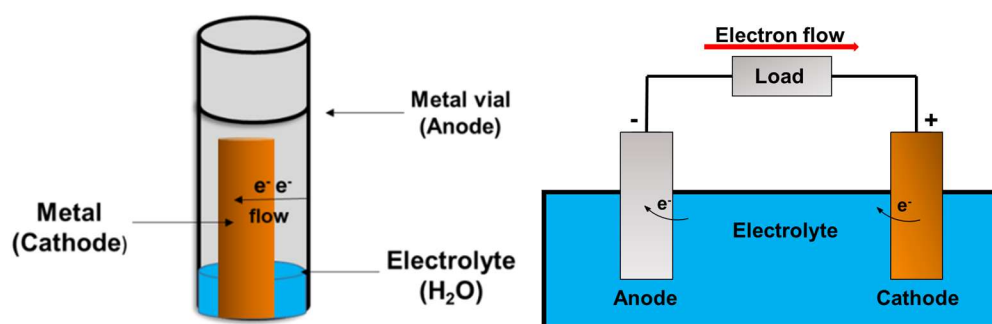


Optimization of electrochemical reduction using S.S vials Via Mechanochemistry

Introduction

Mechanochemistry is an increasingly popular field in chemistry where chemistry is achieved through the use of machines. One of the machines used is the high-speed ball mill. The milling media for this reaction are vials made from different materials like stainless-steel, copper, and PTFE. The reactant and reagents are added to the vial along with the ball bearing to facilitate efficient mixing. This form of chemistry has many advantages, including safety, as the chemist is separated from the reaction. Mechanochemistry offers significant environmental benefits as a small amount/no solvent is needed for the response, resulting in less production of solvent waste. Electrochemistry occurs when you have two different conductive metals immersed in an electrolyte solution, electric current is generated due to the oxidation-reduction reaction that takes place on the electrode surface. One metal undergoes oxidation (anode) while the other undergoes reduction (cathode). The presence of metal vial and metal ball bearing in contact with ionized water as electrolyte resembles the traditional electrochemical cell. Mixed metal combinations are tested in a series to relate the cell potential to reducing specific substrate. The merge between electrochemistry principles with a mechanochemical methodology of high-speed ball milling allowed for the ability to overcome the limitations of each and provide a new tool to carry out chemical reactions.

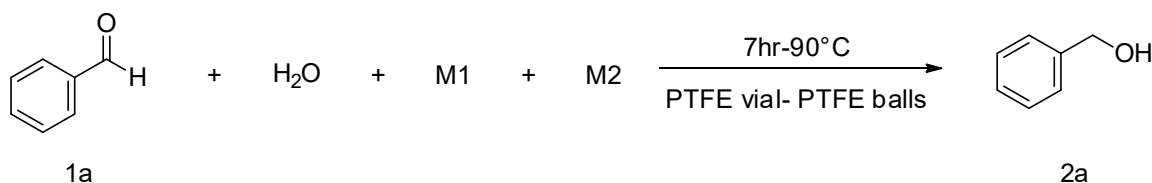


Project objective

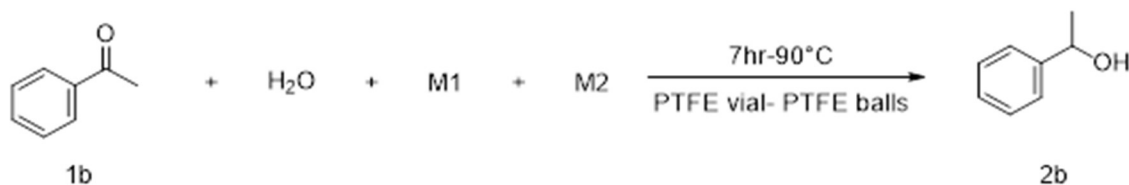
In this research, the metals in stainless steel were being tested for their ability to reduce the substrate successfully. The use of stainless steel metal components electrodes would give an idea of which metals are responsible for reducing organic substrates. Stainless steel is composed mainly of iron, chromium, and nickel. Instead of using S.S vials, PTFE vials/balls were used to eliminate the interference of S.S metal components and to be able to use metal combinations in equal ratios of metals. The use of PTFE vial and balls allow for observation of the role of each of the metals. These metals combinations were tested for the reduction of

acetophenone to alcohol form. The results show the % conversion from each metal combination against the calculated cell potential.

Results and Data



Entry	M1	M2	% Conversion 1a	Calculated cell potential (V)
1	Fe	Cr	>99	0.3
2	Fe	Ni	>99	0.19
3	Cr	Ni	48	0.49



Entry	M1	M2	% Conversion 1a	Calculated cell potential (V)
1	Fe	Cr	5	0.3
2	Fe	Ni	>99	0.19
3	Cr	Ni	4	0.49

Conclusion

The intention was to use electrochemistry principles with a mechanochemical methodology of high-speed ball milling allowed for the ability to overcome the limitation of each. The data for the benzaldehyde reactions in 1a shows that conversion to final product follows the trend of cell potential. The role of chromium was shown in the data for the acetophenone reactions in 1b. This shows that the trend observed in 1a is suppressed by the chromium when it participates in a metal combination. This observation means that the reaction vial that is used to achieve electrochemical reduction could be optimized by having lower ratios of chromium present with higher ratios of iron and nickel. This would allow for greater yield of products in electrochemical reactions done using mechanichemistry.

References

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