XXI Brazilian Meeting on Inorganic Chemistry
X Brazilian Meeting on Rare Earths
III Workshop on Theoretical Bioinorganic Chemistry
Belo Horizonte, September 12 - 15th 2024

Optimization of the catalytic oxidation of benzyl alcohol by iron-tetraphenylporphyrin complex via multivariate analysis

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Thematic Area: Catalysis

Keywords: Metalloporphyrin, benzyl alcohol, multivariate analysis.

Industrially, the conversion of benzyl alcohol (BnOH) into benzaldehyde (BA) and benzoic acid (BzA) is strategically relevant, as BA accounts for more than US$ 330 million in the global market, and is found in various applications in spices, adhesives, dyes and pharmaceuticals[1]. Optimizing reaction conditions to maximize product formation is a crucial step, and a very useful tool for this is the use of multivariate analysis, in which multiple variables are evaluated simultaneously[2]. In view of the difficulties in oxidizing primary alcohols and the growing demand for metal complexes as catalysts, this work aims to evaluate the catalytic performance of an iron(III) complex through a multivariate analysis approach, in which the variables (catalyst concentration and time) are evaluated simultaneously for the homogeneous catalytic oxidation of benzyl alcohol promoted by a porphyrin iron(III) complex. The complex was synthesized and characterized according to methods already described[3]. The catalytic oxidation of BnOH was carried out in CH_2Cl_2, where the optimized variables were catalyst concentration (0.1-5.0 mol%) and time (5-120 min). 2.4 $x10^{-2}$ mmol was used as oxidizing agent. The temperature was kept constant at 20°C. All reactions were monitored by HPLC-DAD and the main products BA and BzA were quantified by means of predetermined calibration curves using toluene as an internal standard. A full factorial design (3k + PC) was used as the response surface methodology, totaling 11 experiments. A response surface was obtained for [time]x[catalyst] using the % conversion of BA and BzA as the obtained data. After statistical analysis, it was possible to obtain optimized values for [catalyst] and reaction time for BA, with 3.5 mol% of catalyst and 120 minutes of reaction, with a conversion of 6.52%. For BzA, the model pointed to higher catalyst concentrations and time (>5.0 mol% and >120 min). Also with the statistical analysis, a tendency was observed for the values obtained, so Figure 1 shows the results with reaction monitoring carried out for the conversion of BnOH into BA in which it was possible to determine the moment when the reaction saturates. The same was done for the formation of BzA at 5.0 and 2.45 mol%, and BzA was not quantified at 0.10 mol%. Future analyses will discuss the effect of variables and their impact on these results.

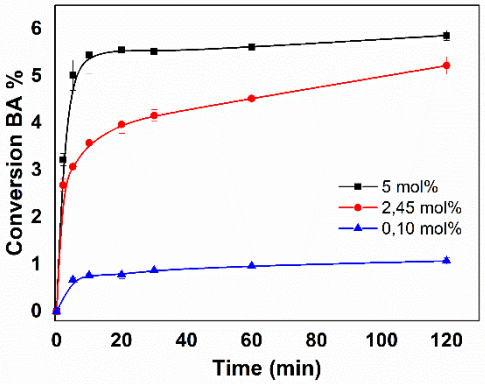

Figure 1 - Reaction monitoring of the catalytic oxidation of BnOH to form BA, mediated by [FeCl(TPP)].

Acknowledgments: CAPES, CMU/UDESC and FAPESC.

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