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

The Determination of Kinetics Parameters for the Oxidation of 3,5-di-*tert*-butylcatechol in the Presence of a Nickel(II) Complex

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Thematic Area: Biological Inorganic Chemistry

Keywords: Catalyst, Oxidative Process, Bioinorganic Chemistry

Oxidative processes are widely spread in many biological systems and play an important role in the survival of the living beings. These types of reactions often need the presence of enzymes to catalyze typical process. Nickel is a common metal found in the active site of metalloenzymes, which generally participates in electron transfer reactions. In this way, bioinorganic chemists search for biomimetic complexes that can catalyze oxidative processes.[1] Tetradentate nitrogenated ligands are usually employed to guarantee the formation of complexes containing labile *cis* sites suitable to the substrate coordination.[2] Therefore, the main goal of this work is evaluate the promiscuity of the nickel(II) complex, $[Ni(bis(1\text{-methylimidazol-2-il})methyl)(2\text{-}(pyridil\text{-}2\text{-}il)ethyl)amine)(H_2O)Cl]ClO_4$, as a catalyst in the oxidation of 3,5-di-*tert*-butylcatechol (3,5-DTBC).[3] This complex has been previously investigated as an electrochemical catalyst for the generation of H_2 and O_2 in water. The complex was synthesized and characterized as previously described.[2] The reactivity was investigated using the reaction with 3,5-DTBC in methanol saturated with O_2 at 25°C. Initially, electronic spectra were recorded in the range of 300 to 1100 nm, at every 30 s, in a methanolic solution containing [Complex] = 1×10^{-5} mol L^{-1} and [3,5-DTBC] = 1×10^{-3} mol L^{-1}, for 30 min. The results shown the formation of the typical band of 3,5-di-*tert*-butyl-*o*-quinone (3,5-DTBQ) at 400 nm. The effect of pH was investigated using different buffer solutions to carry the reaction in the pH range 7.0 – 11.5. As a result, higher activities were observed at the high pH values. The effect of substrate concentration was investigated in the range 0.5×10^{-1} to 5.0×10^{-1} mol L^{-1}, at pH 9.0, and [complex] = 1×10^{-3} mol L^{-1}. The plot of initial rates versus [substrate] shown a Michaelis-Menten curve and the Lineweaver-Burk plot allowed to determine the V_{max} and K_M values as 2.53×10^{-7} mol L^{-1} s^{-1} and 1.31×10^{-3} mol L^{-1}, respectively. Lastly, the effect of the concentration of the complex was investigated in the range 1.0×10^{-4} and 1.0×10^{-3} mol L^{-1} at pH 9.0 and [substrate] = 1.0×10^{-3} mol L^{-1}. As a result, it was observed that the initial rates increase linearly with the concentration of complex, indicating that the reaction follows a first-order behavior regarding the complex concentration. Finally, we conclude that this complex presents the promiscuity ability to catalyze different substrates with environmental interest.

Acknowledgments: CAPES, CNPq, FAPERJ, PIBIC-UFRJ

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