Electrochemical and Theoretical Study of Metronidazole Drug as Inhibitor for Copper Corrosion in Hydrochloric Acid Solution

Adriana Samide^{1,*}, Bogdan Tutunaru¹, Aurelian Dobrițescu^{1,*}, Petru Ilea², Ana-Cristina Vladu^{1,2}
Cristian Tigae¹

¹ University of Craiova, Faculty of Sciences, Department of Chemistry, Calea Bucuresti, 107i, Craiova, Romania

² Babes-Bolyai University, Faculty of Chemistry and Chemical Engineering, Department of Chemical Engineering, Arany Janos Street no. 11, Cluj-Napoca, Romania

*E-mail: samide_adriana@yahoo.com; dobri_aur@yahoo.com

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The approach current trend of expired drugs as corrosion inhibitors for metals and alloys in different environments to avoid its pollution with corrosion products by diminishing the degradation rate of materials is reflected, in our study, by investigation of metronidazole (MNZ) antibiotic and antiprotozoal drug, as corrosion inhibitor for copper in hydrochloric acid solution. The electrochemical measurements associated with UV-Vis spectrophotometry followed by quantum chemical calculations were performed, their results showing that: MNZ inhibition efficiency reached a value of 90.0 % ± 2 , at 1.0 mmol L⁻¹ inhibitor concentration; the amount of corrosion products decreases in the presence of MNZ; the formation of complexes between MNZ and copper, as well as their effective contribution to growth a protective layer at the metal/solution interface; MNZ action mechanism resulted from the parallel processes between the occurrence of chemical bonds and electrostatic interactions was certified by quantum chemical calculations, when *ab initio* to the approximate level of density functional theory (DFT) was used by assigning the Gamees molecular modeling.

Keywords: corrosion inhibition; metronidazole; electrochemical measurements; UV-Vis spectrophotometry; quantum chemical studies

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