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Predicting anti-corrosion properties and modelingnew inhibitors based on the existing variety of organic compounds in relation to low-carbon steel in the media of 1 M hydrochloric acid

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Abstract

In this work, various organic corrosion inhibitors have been selected from the literature [1-28] to be classified by the structure and to compile the base of numerical values of anticorrosive efficiencies (E). For each of the selected compounds by DFT B88-LYP in the basis set 6-31G(d,p) (GGA) (a software *packageCache Work System Pro 7.52*) there were determined the numerical values of the polarizability (α). The data obtained were systematized on the grounds of the organic compounds belonging to certain classes. Then with the use of mathematical methods analytical forms of correlation equations and systems of equations that describe the type of spline approximation «α (axis X) – E (axis Y)» were identified.