The reletionsheip between the structure and activity of some heterocyclic compounds

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This thesis includes four main chapters. The first of which includes an introductory include a review on the organic compounds used as corrosion inhibitors for steel in acidic medium and on the aim of the present study which has been directed towards the ability of the propose methods for the prediction of the corrosion inhibitions of new materials.The second chapter comprises of five parts. The first part describes the quantum chemical parameters of some aniline derivatives (obtained by AM1, PM3, MINDO/3 and MNDO semi-empirical SCF calculations in gas and aqueous phases) correlated to corrosion inhibition efficiency of steel in aqueous acidic medium in order to search for possible correlations between corrosion inhibition efficiency and structural properties as well as to estimate the corrosion inhibition of some related structures. Geometric structures, total negative charge on the molecule (TNC), highest occupied molecular orbital (EHOMO), lowest unoccupied molecular orbital (ELUMO), core-core repulsion (CCR), dipole moment (μ), total energy (TE), and linear solvation energy terms, molecular volume (Vi) and dipolar-polarization (*) were correlated to corrosion inhibition efficiency. The correlation between quantum parameters and experimental inhibition efficiency has been validated by single point calculations for the semiemperical AM1 structures using B3LYP/6-31G* as a higher level of theory. Equations were proposed using linear regression analysis to calculate corrosion inhibition efficiency. The agreement with the experimental data was found to be satisfactory; the standard deviations between the calculated and experimental results ranged between 0.03 to 2.37 and 0.02 to 2.74 for gas phase and aqueous phase, respectively. The inhibition efficiency was closely related to orbital energies ELUMO in most cases. The proposed equations were applied to predict the corrosion inhibition efficiency of some related structures to select molecules of possible activity from a presumably proposed library of compounds.The second part of the second chapter describes an investigation of quantum chemical study of the efficiency of some aromatic hydrazides and Schiff base derivatives containing pyridine, pyrimidine, aminophenylene and salicyaldimine moieties as corrosion inhibitors of steel in presence of 1M HCl. The AM1, PM3, MINDO/3 and MNDO semi-empirical SCF molecular orbital methods were used. A possible correlation between corrosion inhibition efficiencies and structural properties has been deduced. This methodology could reduce the number of compounds to be selected for testing from a library of compounds. Quantum parameters, TNC on the molecule, EHOMO,

ELUMO, μ, TE, and linear solvation energy terms, Vi and * were correlated to corrosion inhibition efficiency of the studied compounds. The results were used to predict the corrosion inhibition of some related aromatic hydrazide derivatives with correlation coefficient r > 0.96.The third part of second chapter includes correlation between quantum chemical SCF calculations of some parameters of benzimidazoles and their inhibition efficiency in case of steel in aqueous acidic medium. Geometric structures, TNC, EHOMO, ELUMO, μ and linear solvation energy terms, Vi and * were correlated to corrosion inhibition efficiency. The correlation between quantum parameters obtained by AM1 calculation and experimental inhibition efficiency has been validated by single point calculations for the semi-empirical AM1 structure using B3LYP/6-31G* as a higher level of theory. Equations were proposed using linear regression analysis to calculate corrosion inhibition efficiency. It was established that the increase of the orbital energies EHOMO favor the inhibition efficiency toward steel corrosion. The proposed linear equations were applied to predict the corrosion inhibition efficiency of some related structures in order to select molecules of possible activity from a library compounds.The fourth part of second chapter investigates the corrosion inhibition efficiencies of some triazole, oxadiazole and thiadiazole derivatives for steel in presence of acidic medium by using AM1, PM3, MINDO/3 and MNDO semi-empirical SCF molecular orbital methods. Geometric structures, TNC, EHOMO, ELUMO, core-core repulsion (CCR), μ and linear solvation energy terms, Vi and *, were correlated to corrosion inhibition efficiency. Four equations were proposed to calculate corrosion inhibition efficiency. The agreement with the experimental data was found to be satisfactory; the standard deviations between the calculated and experimental results ranged between 0.03 and 4.18. The inhibition efficiency was closely related to orbital energies (EHOMO and ELUMO) and μ. The correlation between quantum parameters and experimental inhibition efficiency has been validated by single point calculations for the semiemperical AM1 structures using B3LYP/6-31G** as a higher level of theory. The proposed equations were applied to predict the corrosion inhibition efficiency of some related structures to select molecules of possible activity from a presumable library of compounds.The fifth part of second chapter describes the quantum chemical calculations using the density functional theory (B3LYP/6-31G* DFT) and semi-empirical AM1 methods on 10 pyridine derivatives used as corrosion inhibitors for mild steel in acidic medium to determine the relationship between molecular structure and their inhibition efficiencies. Quantum chemical parameters such as TNC on the molecule, EHOMO, ELUMO and μ as well as linear solvation energy terms, Vi and * were correlated to corrosion inhibition efficiency of ten pyridine derivatives. A possible correlation between corrosion inhibition efficiencies and structural properties was searched to reduce the number of compounds to be selected for testing from a library of compounds. It was found that theoretical data support the experimental results. The results were used to predict the corrosion inhibition of 24 related pyridine derivatives.The third chapter deals with the experimental part of the work. It includes the programs and methods of calculation used in this research work.The fourth chapter is the conclusions which showed the good relation between the quantum chemical parameters and the inhibition efficiency of the studied compounds. It is also showed the importance of this type of

research to predict the inhibition efficiency of predicted new organic compounds as corrosion inhibitors for steel in acidic medium.The thesis included English and Arabic summaries and it is ended by a list of references.