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Corrosion inhibitors part V: QSAR of benzimidazole and 2-substituted derivatives as corrosion inhibitors by using the quantum chemical parameters☆

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Abstract

Quantum chemical SCF calculations of some parameters of benzimidazoles were correlated with their inhibition efficiency in case of steel in aqueous acidic medium. Geometric structures, total negative charge on the molecule (TNC), highest occupied molecular orbital (E_{HOMO}), lowest unoccupied molecular orbital (E_{LUMO}), dipole moment (μ) and linear solvation energy terms, molecular volume (*Vi*) and dipolar-polarization (π^*) 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 E_{HOMO} favors 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.
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Keywords: AM1; B3LYP/6-31G*; Benzimidazole; Corrosion inhibition; Inhibitors; QSAR

1. Introduction

Organic compounds are effective inhibitors of the corrosion of many metals and alloys in aqueous media [1–7]. They reduce corrosion rates of metallic materials in acidic media. Organic compounds having centers for π-electrons and functional groups such as –C=C–, –C≡C–, –OR, –SR and/or $–NR_2$ are the most corrosion inhibitor compounds. The planarity of heterocycles and the presence of a lone pair of electrons on the heteroatoms are important requirements that determine the adsorption of these molecules on the metallic surface [8]. The quantum-chemistry calculations have been widely used to study the reaction mechanisms and to interpret the experimental results as well as to solve chemical reaction ambiguities. The molecular structure and the electronic parameters can be obtained by means of the theoretical calculations by using the computational methodologies of quantum-chemistry.

The objective of this work is to perform a detailed calculation of the molecular structure of benzimidazoles **1**–**5** (Fig. 1) to explore the possible correlations between corrosion inhibition efficiencies and a number of quantum molecular properties such as E_{HOMO}, E_{LUMO}, total negative charge on molecules and linear solvation energy relationship parameters. Thus, a relation between their quantum chemical parameters and their effectiveness as corrosion inhibitors for steel in acidic media could be detected. Then using such relations for prediction of corrosion efficiency for some related structures in order to select the most probable imidazole compounds to be tested as corrosion inhibitors; thus, saving time and more favorable from the economical point of view.

2. Theory and computational details

All computational studies were performed with Restricted Hartree-Fock (RHF) level using AM1 semi-empirical SCF-MO methods in the MOPAC 2000 program and Gaussian 98 with density functional methods [9]. Calculations were performed in

☆ For parts I–IV, see Ref. [1].

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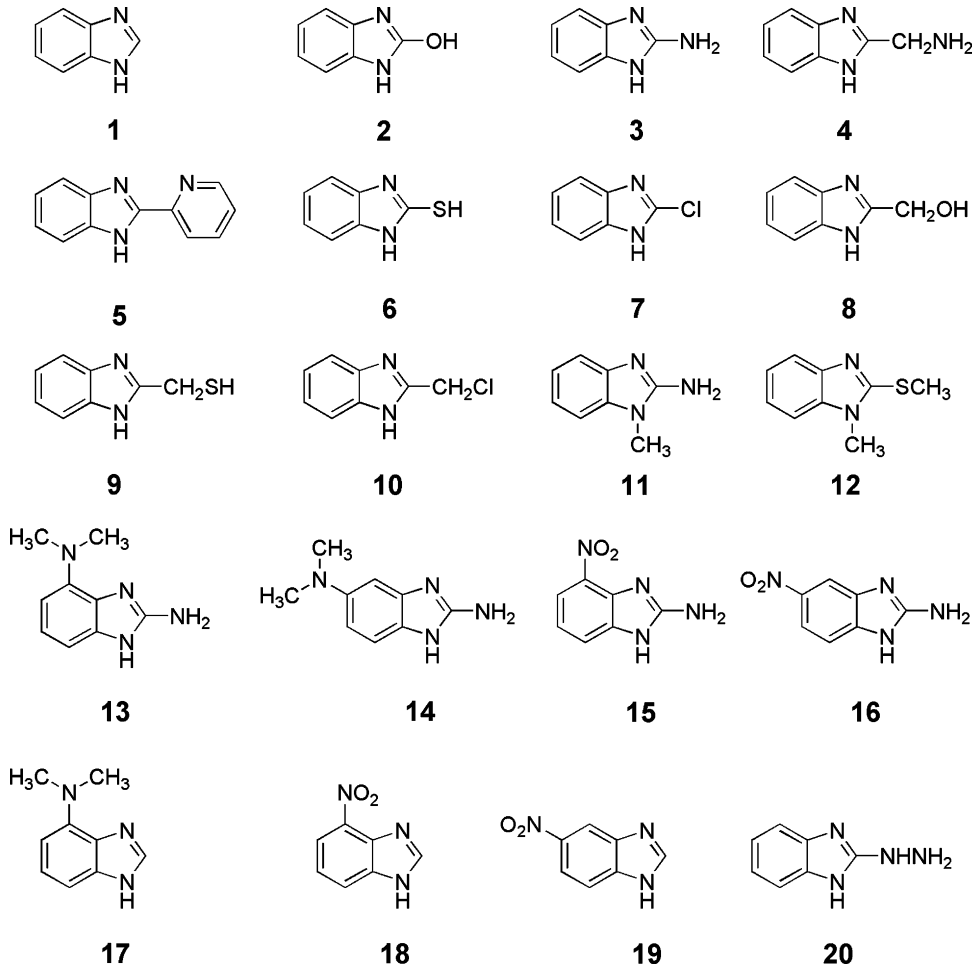

Fig. 1. Structures of compounds **1–20**.

Table 1
Quantum chemical parameters of compounds **1–20** using semi-empirical AM1 calculation in gas phase

Compound no.	*Vi* (cm^3/M)	π^*	Critical volume ($Å^3$/M)	Log *P*	E_{HOMO} (eV)	E_{LUMO} (eV)	E_{L-H} (eV)	μ (Debye)	TNC
1	62.37	1.46	358.5	1.34	−8.996	0.058	9.054	3.139	−0.999
2	66.37	1.91	374.5	1.40	−8.797	0.052	8.849	1.908	−1.226
3	69.17	1.78	387.5	0.99	−8.582	0.057	8.639	2.795	−1.282
4	78.79	1.78	443.5	0.51	−8.933	−0.017	8.916	2.693	−1.333
5	101.03	2.33	579.5	1.95	−8.790	−0.655	8.134	4.526	−1.491
6	73.52	1.81	412.5	1.98	−8.517	−0.124	8.392	1.913	−1.063
7	70.72	1.81	407.5	1.98	−9.074	−0.201	8.873	3.143	−0.903
8	75.98	1.86	433.5	0.89	−8.843	0.059	8.902	2.383	−1.277
9	83.13	1.81	468.5	1.72	−8.927	−0.222	8.704	2.759	−1.130
10	80.33	1.81	463.5	2.11	−9.018	−0.107	8.911	4.004	−1.043
11	78.79	1.93	445.5	1.23	−8.495	0.121	8.616	3.350	−1.303
12	92.75	1.71	485.5	2.47	−8.239	0.009	8.248	2.223	−1.458
13	122.07	1.91	517.5	1.27	−7.803	0.254	8.057	1.103	−1.707
14	122.07	1.91	517.5	1.27	−8.202	0.103	8.305	2.029	−1.641
15	78.39	2.20	444.5	1.05	−9.171	−1.030	8.141	8.279	−1.854
16	78.39	2.20	444.5	1.05	−9.281	−0.907	8.374	8.369	−1.867
17	115.26	1.91	509.5	1.10	−7.785	0.322	8.107	1.457	−1.502
18	78.73	1.90	445.5	0.91	−9.756	−1.119	8.637	8.351	−1.508
19	78.73	1.90	445.5	0.91	−9.809	−0.978	8.831	7.960	−1.565
20	75.98	2.03	422.5	0.51	−8.520	0.114	8.634	3.399	−1.402

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