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Journal of Molecular Structure: THEOCHEM 732 (2005) 173–182

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QSAR study on N-containing corrosion inhibitors: Quantum chemical approach assisted by topological index

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Received 28 October 2004; accepted 28 February 2005
Available online 8 September 2005

Abstract

In this paper, QSAR study on N-containing corrosion inhibitors has been made using quantum chemical approach assisted by a novel topological index ($^2X^{v\#}$). Two models were obtained and their efficiency was examined using statistics. The results indicate that inhibition efficiencies relate to some parameters of corrosion inhibitors, such as E_{homo}, polarizability, Dipole, frontier orbital charge density, the interaction mode between inhibitors and metal surface (feedback donor–acceptor coordination bonds), $^2X^{v\#}$ (steric hindrance of molecules). Predicted values are consistent with the experimental ones on the whole. The residuals range within the experimental error. So the models can be used to predict inhibition efficiencies of the same type molecules.

Keywords: N-containing corrosion inhibitors; QSAR; Quantum chemical approach; Topological index; Inhibition efficiency

1. Introduction

The working mechanism of corrosion inhibitors is a crucial problem for anti-corrosion researchers, but it has not been managed to consensus up to now. Theoretical studies carried out in this area get far behind the experimental research [1–4]. The synthesis and selection of corrosion inhibitors are still based on trial-and-error experimentation. Hence, it is urgent to investigate corrosion inhibition mechanism and the influence of the substituted group on inhibition efficiency in theory. It will provide theoretic guidance for the design of corrosion inhibitors.

As we know, some organic compounds containing hetero atom, such as O, N, or S, with free electron pairs which are readily available for sharing, are found to be effective corrosion inhibitors for many metals and alloys [5]. It has been commonly recognized that feedback coordinate covalent bonds formed between organic inhibitor and metal surface during chemical adsorption process [6]. Imidazole, benzimidazole, and their derivatives studied in this paper are organic inhibitors with these characteristics. They can form an even film on transitional metal surface instantaneously, thereby reducing the corrosive attack of metals in acidic media [5,7].

The relationships between descriptors characterizing the structure properties of chemicals on quantitative basis are structure–activity relationships (QSAR). It correlates and predicts physical and chemical properties of chemicals, plays an important role in effective assessment of organic compounds. The application of QSAR in corrosion research has been reported [8–13].

Quantum chemical calculation has been widely used to study reaction mechanism. It also proved to be a very powerful tool for studying inhibition mechanism [8–10,14–16]. The relationships between structural parameters, such as electronic properties of inhibitors, the frontier molecular orbital energy (E_{homo}, E_{lumo}) and the hydrophobic /hydrophilic nature, the charge distribution of the studied inhibitors and their inhibition efficiencies were investigated in these studies. Quantum chemical descriptors have obvious advantages, they are not restricted closely to related compounds, as is often the case with group theoretical, topological and others, and they make interpretation of QSAR equations more straightforward. In addition, they were obtained without laboratory measurements, thus saving time and equipment, alleviating safety and disposal concerns.

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0166-1280/$ - see front matter © 2005 Elsevier B.V. All rights reserved.
doi:10.1016/j.theochem.2005.02.091

Molecular connectivity index (MCI), a topological property based on use of mathematical characterization of compounds in contrast to physico-chemical characterizations traditional, was proposed by Kier et al. [17]. It reveals the figured characteristics and steric hindrance effect of molecule. MCI is as complementary [18] to the prevailing approaches of the past based on use of selected properties as descriptors, because previous literatures on the QSAR study of corrosion inhibitors confined to quantum chemical calculation, whereas the steric hindrance effect of molecules (MCI) had scarcely been taken into account. Zhao et al. studied the inhibition efficiencies of imidazole derivatives, including 2-phenylimidazole and 2-ethyl-4-methylimidazole, which display distinct steric hindrance effect. They found that the multiple correlation coefficient (R^2) of the equation between inhibition efficiencies and parameters was too poor to be accepted without MCI, whereas it would be improved greatly when the MCI was included. So MCI is crucial to QSAR study especially for those molecules that show distinct steric hindrance. Our paper will study

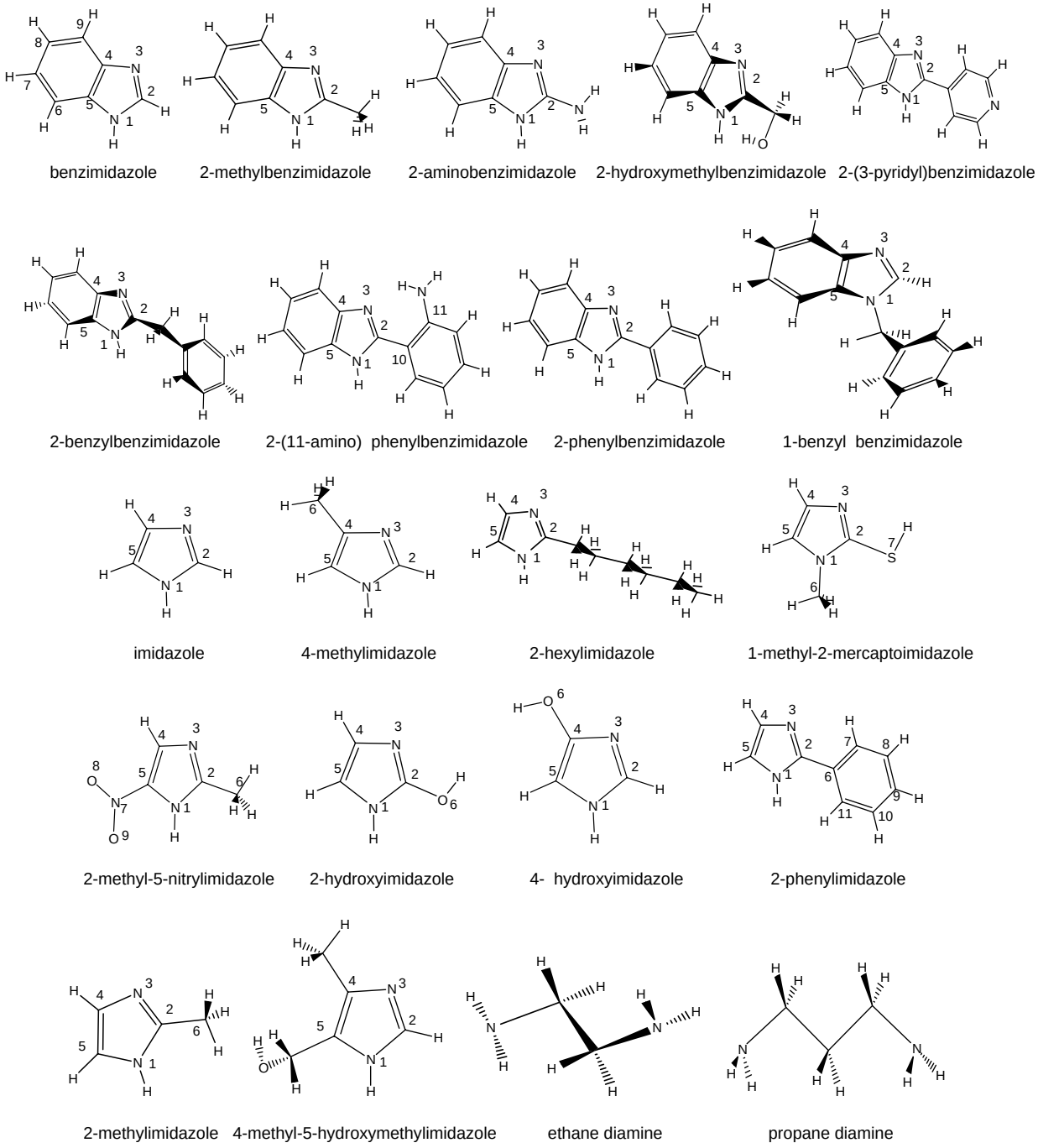

Fig. 1. The optimum structure of 34 corrosion inhibitors.