ABSTRAK

STUDI *AB INITIO* SENYAWA INHIBITOR KOROSI 2-FENILIMIDAZOL[1,2-α]PIRIDIN, 6-METIL 2-FENILIMIDAZOL[1,2α]PIRIDIN, 6-METIL-2-(4-METOKSIFENILIMIDAZOL)[1,2α]PIRIDIN DAN 6-METIL-2-(4-KLOROFENILIMIDAZOL)[1,2α]PIRIDIN

Senyawa imidazol dan beberapa turunannya telah dikenal sebagai senyawa yang dapat menjadi inhibitor korosi. Pada penelitian ini, dilakukan perhitungan *ab-initio* untuk senyawa 2-fenilimidazol[1,2-α]piridin, 6-metil-2-fenilimidazol [1,2α]piridin, 6-metil-2-(4-metoksifenilimidazol)[1,2α]piridin, dan 6-metil-2-(4-klorofenilimidazol)[1,2α]piridin. Perhitungan dilakukan untuk mengetahui sifat elektronik senyawa-senyawa tersebut dan korelasinya dengan efisiensi inhibisi korosi. Perhitungan dilakukan dengan menggunakan perangkat lunak *Firefly*. Dari hasil perhitungan secara komputasi, diketahui bahwa senyawa 6-metil-2-(4-metoksifenilimidazol)[1,2α]piridin lebih berpotensi sebagai inhibitor korosi yang baik dibandingkan senyawa yang lainnya, karena memiliki celah energi, potensial ionisasi, afinitas elektron, elektronegativitas dan *global hardness* paling rendah yaitu masing-masing 10,184 eV, 7,199 eV, -2,985 eV, 2,107 eV dan 5,092 eV serta *global softness* paling tinggi yaitu 0,098 eV Sedangkan nilai momen dipol terbesar dimiliki oleh senyawa 6-metil-2-(4-klorofenilimidazol)[1,2α]piridin yaitu 6,125 Debye, karena atom Cl kepolarannya lebih besar dibandingkan gugus substituen yang lain.

Kata-kata kunci: *ab initio*; adsorpsi; korosi; inhibitor korosi; imidazol; turunan imidazol.

ABSTRACT

AB INITIO STUDY OF CORROSION INHIBITOR COMPOUNDS 2-PHENYLIMIDAZOLE[1,2-α]PYRIDINE, 6-METHYL-2-PHENYLIMIDAZOLE[1,2-α]PYRIDINE, 6-METHYL-2-(4-METHOXYPHENYLIMIDAZOLE)[1,2-α]PYRIDINE AND 6-METHYL-2-(4-CHLOROPHENYLIMIDAZOLE)[1,2-α]PYRIDINE

Imidazole compounds and some of its derivatives have been known as a compound which can be used as corrosion inhibitor. In this study, ab initio calculations for 2-phenylimidazole[1,2-α]pyridine, 6-methyl-2-phenylimidazole[1,2-α]pyridine, 6-methyl-2-(4-methoxyphenylimidazole)[1,2-α]pyridine, and 6-methyl-2-(4-chlorophenylimidazole)[1,2α]pyridine was carried out. The calculation was carried out to determine the electronic properties of these compounds and their correlation with corrosion inhibition efficiency. Calculations were performed using the Firefly software package. From the computational calculation results, it was found that 6-methyl-2-(4-metoxyphenylimidazole)[1,2α]pyridine compound has better potential as a corrosion inhibitor compounds than the rest of the compounds due to its small energy gap, low ionization potential, low electron affinity, low electronegativity and low global hardness with values of 10.184 eV, 7.199 eV, -2.985 eV, 2.107 eV and 5.092 eV respectively. This compound also has the highest global softness of 0.098 eV, while the greatest value of the dipole moment was possessed by 6-methyl-2-(4-chlorophenylimidazole)[1,2α]pyridine with value of 6.125 Debye due to the polarity of Cl atom that is larger than the other substituent groups.

Keywords: ab initio; adsorption; corrosion; corrosion inhibitor; imidazole; imidazole derivative.