MEMPELAJARI EFISIENSI INHIBISI KOROSI SENYAWA *XANTHONE* DAN TURUNANNYA PADA LOGAM FE MENGGUNAKAN METODE *DENSITY FUNGSIONAL THEORY* (DFT)

TESIS

FITRIA RAMADHANI
NIM. 1720412017

Pembimbing I : Prof. Dr. Emriadi
Pembimbing II : Dr. Syukri

PROGRAM STUDI MAGISTER KIMIA
JURUSAN KIMIA FAKULTAS MIPA
UNIVERSITAS ANDALAS
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Mempelajari Efisiensi Inhibisi Korosi Senyawa *Xanthone* Dan Turunannya Pada Logam Fe Menggunakan Metode *Density Fungsional Theory* (DFT)

Oleh: Fitria Ramadhani (1720412017)

(Dibawah bimbingan: Prof. Emriadi dan Dr. Syukri)

Abstrak

Potensi sifat inhibitor korosi dari senyawa *xanthone* dan turunannya (*gartanin, 8-desoxygartanin, α-mangostine,* dan *β-mangostine*) dapat dibuktikan melalui teori fungsional kerapatan (DFT) pada tingkatan teori B3LYP/6-31G(d,p). Parameter kimia kuantum seperti energi orbital molekul tertinggi yang diduduki elektron (E_{HOMO}), energi orbital molekul terendah yang tidak diduduki elektron (E_{LUMO}), celah energi (E_{gap} / ΔE), momen dipol (μ), dan energi total (E_{tot}) dapat dihitung mengunakan metode DFT. Persamaan analisis data DFT dapat menentukan nilai; energi potensial (I), afinitas elektron (A), elektronegativitas absolut (χ), *hardness* global (η), *softness* global (σ), jumlah elektron transfer (ΔN), elektrofilisitas (ω), dan efisiensi inhibisi korosi (IE%). Hasil perhitungan parameter kimia kuantum menunjukkan potensi sifat inhibitor dari *gartanin* > *α-mangostine* > *β-mangostine* > *8-desoxygartanin* > *xanthone*, dengan nilai efisiensi inhibisi korosi terhitung dari *gartanin* adalah sebesar 86,54%.

Inhibitor *gartanin* divariasikan dengan penambahan subtituen, didapatkan pada penambahan subtituen NH_2 lebih baik dibandingkan dengan penambahan subtituen lainnya. Nilai efisiensi inhibitor yang didapatkan dari *gar-*NH_2 adalah 92,91%. Senyawa gartanin sebagai inhibitor diinteraksikan dengan logam Fe, didapatkan kemungkinan posisi terbaik antara inhibitor dan logam Fe adalah posisi 1 dan 6.

Kata kunci: DFT, inhibitor korosi, *Xanthone*, turunan *Xanthone*, efisiensi inhibitor.

Studying the Corrosion Inhibition Efficiency of Xanthone Compounds and Derivatives in Fe Metals Using Theory Functional Density Method (DFT)

By: Fitria Ramadhani (1720412017)
(Supervised : Prof. Emriadi and Dr. Syukri)

Abstract

Potential corrosion inhibitor properties of xanthone and its derivatives (*gartanin, 8-desoxygartanin, α-mangostine*, dan *β-mangostine*) have been performed using functional density theory (DFT) at the B3LYP / 6-31G (d, p) level of theory. Quantum chemical parameters such as the energy of the highest occupied molecular orbitals (E_{HOMO}), the energy of lowest unoccupied molecular orbital (E_{LUMO}), the energy gap (E_{gap} / ΔE), dipole moment (μ), and total energy (E_{tot}) are calculated by DFT method. Equation analysis of DFT data could determine the value of potential energy (I), electron affinity (A), electronegativity (χ), global hardness (η), global softness (σ), transfer electron number (ΔN), electropilicity (ω), and corrosion inhibitor efficiency (IE%). Quantum chemical parameters showed potential corrosion inhibitor properties of gartanin > α-mangostine > β-mangostine > 8-desoxygartanin > xanthone, with the calculated corrosion inhibitor efficiency of gartanin is 86.54%.

Based on the value of corrosion inhibitor efficiency, the percentage of gartanin was 86.54%. Gartanin inhibitors were varied by the addition of substituents, obtained by adding of NH_2 subtituents better than the addition of other substituents. The inhibitor efficiency value obtained from NH_2-gar was 92.91%. Gartanin compounds as inhibitors are interacted with Fe metal; and it is found that the best position between inhibitors and Fe metals is positions 1 and 6.

Keywords: DFT, corrosion inhibitors, Xanthones, Xanthones derivatives, inhibitor efficiency.