SUPPORTING INFORMATIONS

Adsorption and anticorrosive behavior of aromatic epoxy monomers on carbon steel corrosion in acidic solution: Computational studies sustained experimental studies

Omar Dagdag¹, Zaki Safi², Hamid Erramli³, Omar Cherkaoui⁴, Nuha Wazzan⁵, Lei Guo⁶,

Chandrabhan Verma ^{7,8*}, E. E. Ebenso ^{7,8*} and Ahmed El Harfi ¹

¹Laboratory of Agroresources, Polymers and Process Engineering (LAPPE), Department of Chemistry, Faculty of Science, Ibn Tofail University, BP 133, 14000 Kenitra, Morocco.

²Al Azhar University-Gaza, Chemistry Department, Faculty of Science, P.O Box 1277, Gaza, Palestine

³Laboratory of Materials, Electrochemistry and Environment, Department of Chemistry, Faculty of Sciences, Ibn Tofail University, Kenitra, Morocco.

⁴Higher School of Textile and Clothing Industries, Laboratory REMTEX, BP 7731, Oulfa, Casablanca, Morocco.

⁵King Abdulaziz University, Chemistry Department, Faculty of Science, P.O Box 42805, Jeddah, 21589, Saudi Arabia.

⁶School of Materials and Chemical Engineering, Tongren University, Tongren, 554300, China.

⁷Material Science Innovation & Modelling (MaSIM) Research Focus Area, Faculty of Natural and Agricultural Sciences, North-West University, Private Bag X2046, Mmabatho 2735, South Africa

⁸Department of Chemistry, Faculty of Natural and Agricultural Sciences, School of Chemical and Physical Sciences, North-West University, Private Bag X2046, Mmabatho 2735, South Africa.

*Corresponding author E-mail: chandraverma.rs.apc@itbhu.ac.in, Eno.Ebenso@nwu.ac.za

Supplementary Information



Fig. SI 1.ATR-FTIR spectra of AEM1and AEM2



Fig. SI2.¹H and ¹³C NMR spectra of AEM1and AEM2



Fig. SI3.Plot of the Langmuir adsorption isotherm of aromatic epoxy monomers AEM1 and AEM2 on the carbon steel surface at 298 K.



Fig. SI4.Potentiodynamic polarization curves of carbon steel in 1 M HCl solution in the presence of 10⁻³ M of AEM1 and AEM2 at different temperatures



Fig. SI5.Arrhenius plots of Ln (i_{corr})vs. 1/Tand Ln (i_{corr} /T)vs. 1/T for carbon steel in 1 M HCl solution in the absence and presence of 10⁻³ M AEM1 and AEM2.

Tables

Table SI 1Langmuir adsorption parameters.

Inh	R^2	slope	$K_{\rm ads} ({ m M}^{-1} imes 10^6)$	$-\Delta G_{ads}$ (kJ.mol ⁻¹)
AEM1	0.9999	1.0662	0.42	42.03
AEM2	0.9999	1.0762	1.01	44.20

Table SI 2Influence of temperature on the corrosion rate and inhibition efficiency of carbon steel in1 M HCl at 10⁻³ M of AEM1 and AEM2.

T (K)	E _{corr}		<i>i</i> _{corr}		Ect
		mV/SCE		μA/Cm ²	%
	Blank	10 ⁻³ M of AEM1	Blank	10 ⁻³ M of AEM1	-
298	- 473	-444	916	058.96	93.6
308	- 459	-528	1390	124.40	91.0
318	- 455	-454	2700	219.90	91.8
328	- 453	-537	4100	416.01	89.8
	Blank	10 ⁻³ M of AEM2	Blank	10 ⁻³ M of AEM2	-
298	- 473	-451	916	032.88	96.4
308	- 459	-456	1390	102.00	92.6
318	- 455	-458	2700	216.59	91.9
328	- 453	-468	4100	401.86	90.1

 Table SI 3Activation parameters for carbonsteel in 1 M HCl solution in the absence and presence of AEM2.

	R ²	E _a (kJ/mol)	ΔH _a (kJ/mol)	ΔS _a (J.mol ⁻¹ K ⁻¹)	E _a -ΔH _a (kJ/mol)
Blank	0.9830	41.90	39.30	- 56.70	2.59
10 ⁻³ M of AEM1	0.9977	52.28	49.69	11.97	2.59

10 ⁻³ M of AEM2	0.9790	67.37	64.78	58.49	2.59