Corrosion Inhibition of Mild Steel by Polyaromatic Diimine Derivatives: A Theoretical and Experimental Study

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Aromatic imines based on polyanilines have shown exceptional properties in corrosion inhibiting coatings and as organic semiconductor materials. Presented here is the investigation of electronic and potential anticorrosion properties of a set of aromatic diimines AQ1 to AQ12 derived from the condensation of aniline derivatives with anthraquinone. The electronic properties (e.g. E_{HOMO}, E_{LUMO} and Egap) were studied by computational methods at the DFT level and by the measurement of red/ox potentials (cyclic voltammetry) and optical gaps (absorption spectroscopy). Both, theoretical and experimental values were in good agreement and the results predicted that compounds AQ3 and AQ4 are the most promising diimines for corrosion protection. Consequently, the potential of AQ3 and AQ4 as inhibitor coating was tested on mild steel by potentiodynamic polarization corrosion measurements. Both compounds significantly increased the corrosion resistance of mild steel in aqueous 3.5% NaCl solution but diimine AQ4 was more effective than AQ3.

AQ1: $R_{2\text{-}6}$ = H;
AQ2: $R_{3,5}$ = CH_3, $R_{2,4,6}$ = H;
AQ3: $R_{3,4,5}$ = $OC_{12}H_{25}$, $R_{2,6}$ = H;
AQ4: R_4 = NHPh, $R_{2,3,5,6}$ = H;
AQ5: R_4 = F, $R_{2,3,5,6}$ = H;
AQ6: R_4 = CN, $R_{2,3,5,6}$ = H;
AQ7: $R_{2\text{-}6}$ = F;
AQ8: R_4 = SCH_3, $R_{2,3,5,6}$ = H;
AQ9: R_4 = CO_2CH_3, $R_{2,3,5,6}$ = H;
AQ10: R_4 = SO_2CH_3, $R_{2,3,5,6}$ = H;
AQ11: R_4 = NO_2, $R_{2,3,5,6}$ = H;
AQ12: R_4 = SF_5, $R_{2,3,5,6}$ = H