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Synergistic inhibitive effect and related quantum chemical parameters of 2-ethoxy-4,6-dimethylnicotinonitrile and iodide ions on corrosion of mild steel in sulfuric acid

Punita Mourya, R B Rastogi and M M Singh
Indian Institute of Technology (Banaras Hindu University), India

The effect of iodide ions on the inhibitive performance of 2-ethoxy-4,6-dimethylnicotinonitrile (EDNN) in 0.5 M H₂SO₄ for mild steel (MS) corrosion has been studied using gravimetric, electrochemical impedance spectroscopy (EIS) and potentiodynamic polarization measurements. EDNN inhibits the corrosion of MS and its inhibition efficiency increases on increasing the concentration of the inhibitor at 298 K. The adsorption of EDNN on MS leading to inhibition was found to follow the Langmuir adsorption isotherm. The inhibition efficiency of EDNN increased on the addition of 2.0 mM KI. The synergistic effect of KI was determined by calculating the synergism parameters. The value of synergism parameter which is more than unity indicates the fact that the enhanced inhibition efficiency in the presence of iodide ions is only due to synergism. This synergism showed that a cooperative mechanism exists between the iodide anion and EDNN cations. The increase in surface coverage in the presence of iodide ions indicates that iodide ions enhance the adsorption of EDNN on the negatively charged metal surface. Surface morphology of corroded / inhibited MS has been studied by scanning electron microscopy (SEM) and atomic force microscopy (AFM). X-ray photoelectron spectroscopy (XPS) of the inhibited MS surface has been carried out to determine the composition of the adsorbed surface film. Some quantum chemical parameters and the Mulliken charge densities for EDNN were calculated by the density functional theory (DFT) method to provide further insight into the mechanism of inhibition of the corrosion process.

Biography

Punita Mourya received the B.Sc. degree and M.Sc. degree from Veer Bahadur Singh Purvanchal University, Jaunpur, Uttar Pradesh, India, in 2007 and 2009, respectively. She is currently working towards the Ph.D. degree in the Department of Chemistry, Indian Institute of Technology (Banaras Hindu University), Varanasi, India. She is the senior research fellow of the UGC, India. She has five publications in international journals. Her present research interests include inhibition of acid corrosion of mild steel using heterocyclic organic compounds.

mouryapunita025@gmail.com

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