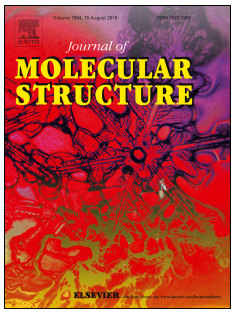
Accepted Manuscript



Synthesis, crystal structure, DFT, molecular dynamics simulation and evaluation of the anticorrosion performance of a new pyrazolotriazole derivative

Youness El Bakri, Lei Guo, El Hassane Anouar, Abdallah Harmaoui, Abdelkader Ben Ali, El Mokhtar Essassi, Joel T. Mague

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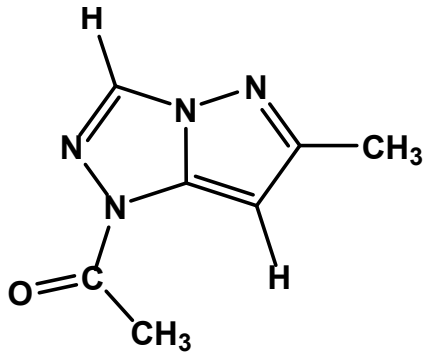

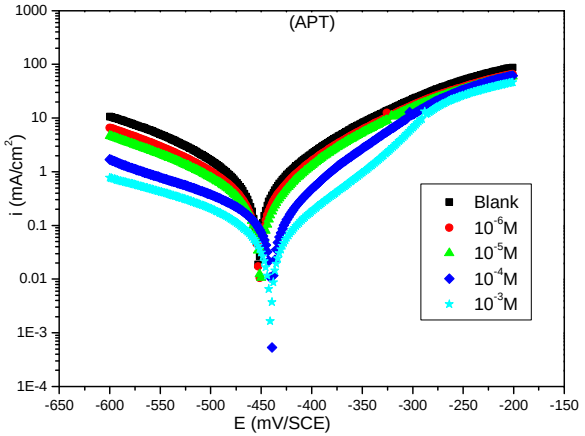

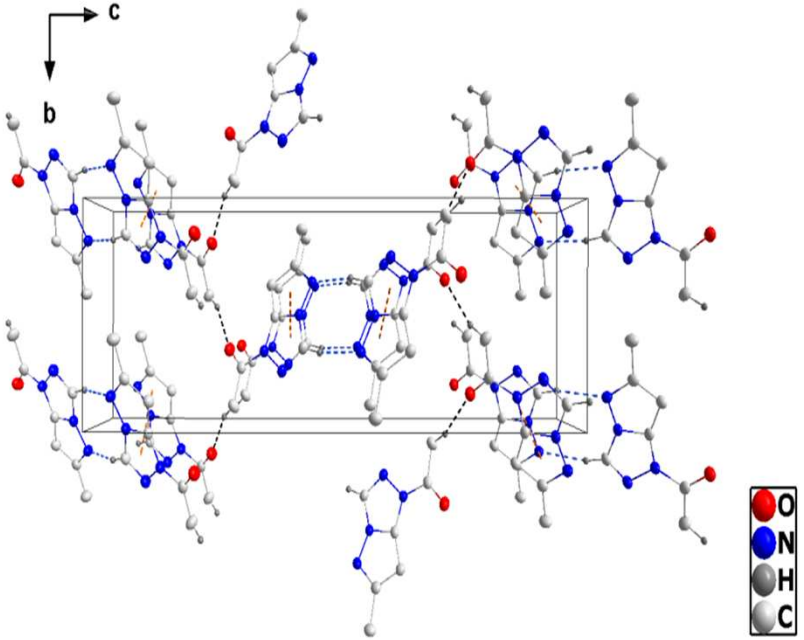

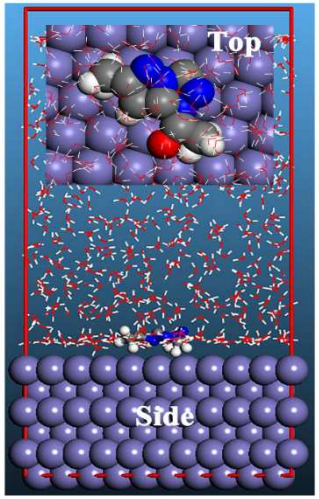

2D structure (up right), molecular packing (bottom right), Polarization curves for carbon steel in the absence (blank) and presence of APT at different concentrations (up left) and MD simulation of APT on Fe surface (bottom left).