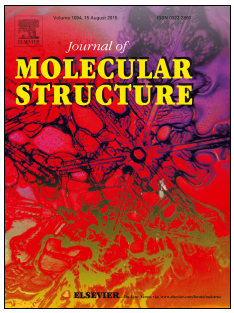
Accepted Manuscript



Synthesis, characterization and computational chemical study of novel pyrazole derivatives as anticorrosion and antiscalant agents

F. El-Taib Heakal, S.K. Attia, S.A. Rizk, M.A. Abou Essa, A.E. Elkholy

PII: S0022-2860(17)30927-4

DOI: 10.1016/j.molstruc.2017.07.006

Reference: MOLSTR 24033

To appear in: *Journal of Molecular Structure*

Received Date: 24 May 2017

Revised Date: 5 July 2017

Accepted Date: 6 July 2017

Please cite this article as: F. El-Taib Heakal, S.K. Attia, S.A. Rizk, M.A. Abou Essa, A.E. Elkholy, Synthesis, characterization and computational chemical study of novel pyrazole derivatives as anticorrosion and antiscalant agents, *Journal of Molecular Structure* (2017), doi: 10.1016/j.molstruc.2017.07.006.

Synthesis, characterization and computational chemical study of novel pyrazole derivatives as anticorrosion and antiscalant agents

F. El-Taib Heakal[a], S.K. Attia[b], S.A. Rizk[c], M.A. Abou Essa[a], A.E. Elkholy[b*]

[a]*Chemistry Department, Faculty of Science, Cairo University, 12613 Giza, Egypt*

[b]*Department of Analysis and Evaluation, Egyptian Petroleum Research Institute, 11727 Cairo, Egypt*

[c]*Department of Chemistry, Faculty of Science, Ain Shams University, 11566 Cairo, Egypt*

Abstract

Metals corrosion and scales deposition are two serious problems of heavy burden in most industries. Both problems can be mitigated by adding special chemicals capable of being adsorbed on metallic surfaces as well as on scale growing crystal surfaces. Efficient materials should be rich in functional groups containing heteroatoms and/or π bonds for supporting their adsorbability on surfaces. In the present work, four novel pyrazole derivatives were synthesized and characterized for their structures using elemental analysis and spectroscopic tools. The tested compounds were fabricated by treating 2,3-diaryloxirane-2,3-dicarbonitriles with different nitrogen nucleophiles. The density functional theory (DFT) was then applied to explore the structural and electronic characteristics of these materials. Molecular dynamics simulation was also run to scrutinize the ability of the prepared compounds to act as corrosion inhibitors and antiscalant agents by adsorbing on Fe and $CaSO_4$ surfaces.

Keywords: Corrosion inhibitors; Antiscalants; DFT; Fukui indices; Molecular dynamics; Pyrazole derivatives.

[*]Corresponding author. Tel.: +20 01115619254; 010024350142

E-mail address: aymanesmat2015@gmail.com; aymanesmat2015@epri.sci.eg