



## Removal of iron (II) from wastewater in oil field using 3-(*p*-methyl) phenyl-5-thionyl-1,2,4-triazoline assembled on silver nanoparticles

Eid M.S. Azzam<sup>a,\*</sup>, Sayed A. Ahmed<sup>b</sup>, Hussein H. Mohamed<sup>b</sup>, Mohamed A. Adly<sup>b</sup>, Elshafie A.M. Gad<sup>a</sup>

<sup>a</sup>Applied Surfactants Laboratory, Petrochemicals Department, Egyptian Petroleum Research Institute, Nasr City, 11727 Cairo, Egypt, Tel. +20 1117710207; emails: eazzamep@yahoo.com (E.M.S. Azzam), eamgad\_99@hotmail.com (E.A.M. Gad)

<sup>b</sup>Department of Chemistry, Faculty of Science, Beni-Suef University, 62514 Beni-Suef City, Egypt, emails: skader\_70@yahoo.com (S.A. Ahmed), h\_gendy\_2010@yahoo.com (H.H. Mohamed), Mohamed.Atia@khalda-eg.com (M.A. Adly)

Received 30 March 2018; Accepted 2 November 2018

---

### ABSTRACT

In this work, we prepared 3-(*p*-methyl) phenyl-5-thionyl-1,2,4-triazoline (C1). The nanostructure of the prepared C1 compound was fabricated by assembling on silver nanoparticles (AgNPs). The ultra-violet and transmission electron microscope analyses confirm the assembling of the C1 compound on AgNPs. The effects of the C1 compound on the removal of iron (II) from iron-contaminated samples (prepared in the laboratory) and industrial wastewater samples (produced water from oil processing facility) were studied before and after their assembling on AgNPs. The removal of iron was studied at different concentrations of FeSO<sub>4</sub> solution (5, 14, and 39 mg/L), and field sample concentration was 661 mg/L. In addition, the removal of iron (II) was investigated at different times. The prepared compound shows high efficiency in removing the iron ions from the used water samples. The AgNPs have a good role in enhancing the removal of iron ions from the water samples. Quantum chemical descriptors using density function theory with the nonlocal correlation functional B3LYP with 6-311G++(p,d) basis set implemented in Gaussian 09 program were  $E_{\text{HOMO}}$  and  $E_{\text{LUMO}}$ . The output of the study pronounces that the C1 molecule can act as a chelating agent for iron (II).

**Keywords:** Triazole derivatives; Silver nanoparticles; Iron (II); DFT; Oil field

---

\* Corresponding author.