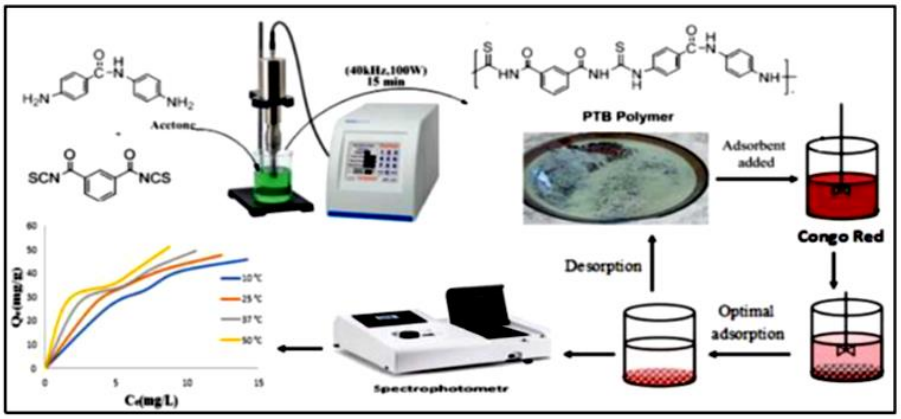
Moroccan Journal of Chemistry
ISSN : 2351-812X

Mor. J. Chem., 2025, Volume 13, Issue 1, Page 325-345
https://revues.imist.ma/index.php/morjchem
https://doi.org/10.48317/IMIST.PRSM/morjchem-v13i1.49505

Sonochemical synthesis of new poly(Thiourea-Amide) as an efficient adsorbent for Congo Red: Adsorptive and DFT studies

Wisam A. Radhi [1, 2,*], Tariq E. Jasim [1], Ahmed M. Jassem [1,]**

[1] *Department of Chemistry, College of Education for Pure Sciences, University of Basrah, Basrah, Iraq*
[2] *Department of Chemistry, Polymer Research Center, University of Basrah, Basrah, Iraq*
* *Corresponding author: Email address: wisam.radhi@uobasrah.edu.iq*
** *Corresponding author: Email address: ahmed.majedd@uobasrah.edu.iq*



Received *11 June 2024,*
Revised *30 Sept 2024,*
Accepted *05 Nov 2024*

Citation*: Radhi W. A., Jasim T. E., Jassem A. M. (2025) Sonochemical synthesis of new poly(Thiourea-Amide) as an efficient adsorbent for Congo Red: Adsorptive and DFT studies, Mor. J. Chem., 13(1), 325-345*

Abstract: In this work, a sonochemical synthesis of new polymer, that is poly(N^1-ethanethioyl-N^3-((4-((4-(methylamino)phenyl)carbamoyl)phenyl)carbamothioyl) isophthalamide) (PTB) from a condensation reaction of isophthaloyl diisothiocyanate and 4,4'-diaminobenzanilide has been developed. Different techniques were utilized to elucidate the chemical structure of the synthesized polymer including FT-IR, 1HNMR, thermal gravimetric analysis (TGA), Brunauer-Emmett-Teller (BET), and field emission scanning electron microscopy (FESEM). The adsorptive performance of the synthesized polymer to adsorb Congo red (CR) dye from an aqueous solution was analytically assessed. Several effective parameters including contact time, pH, adsorbate concentration, adsorbent dose, and temperature on the adsorption process by the target polymer were extensively investigated. The results revealed that the optimal adsorption pH was about 5 with removal efficiency of 83.181% and the adsorbed amount of CR dye increased when environmental temperature was increased. The adsorption isotherms analyses indicated that the Langmuir model was the most relevant to describe the adsorption process compared with the Freundlich model. The study of adsorption kinetics showed that the adsorption model of CR dye onto the polymer surface correlated with a pseudo-second-order model. Based on the thermodynamic studies, the calculated ΔG was negative, ΔH was endothermic, and ΔS was positive, confirming the occurrence of adsorption process is spontaneous. DFT-assisted calculations were performed to identify several important parameters including chemical hardness, electronic chemical potential, electrophilicity, and ΔE_{gap} (E_{HOMO} - E_{LUMO}). These parameters are used as efficient descriptors for evaluating the potential interactions for the selected molecules and their reactivity for adsorption process onto the synthesized polymer (PTB).

Keywords: *Ultrasonic synthesis; Adsorption process; CR dye; Poly(Thiourea-Amide); DFT*