Synthesis of thiosemicarbazone-based colorimetric chemosensor for Cu2+ ions' recognition in aqueous medium: Experimental and theoretical studies

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Abstract

A highly sensitive and selective colorimetric test using an organic compound, namely 2-acetylpyrrole thiosemicarbazone (APT), for the efficient recognition of Cu2+ ions in an aqueous medium has been successfully developed. The optimization of APT in acting as a colorimetric chemosensor was studied using UV-vis spectroscopy. The developed chemosensor in DMSO/Tris-HCl, 1:1, v/v, buffer pH 7 did not show any interference from 15 different metal ions. The limit of detection of the probe for Cu2+ was 19.7 mu M. DMSO showed favourable pairing with APT as a medium for APT to act as a chemosensor, as calculated using the COSMO-RS method. Molecular electrostatic potential, Fukui function and time-dependent-DFT (TD-DFT) were successfully performed to characterize and support the experimental data in predicting the interaction that occurs between APT and Cu2+ ions. The NCI-RDG program showed that a non-covalent interaction formed

between APT and Cu2+ in acting as a chemosensor. Using naked eye observation, the developed APT test strips also successfully recognized Cu2+ ions in different types of spiked water samples. (C) 2020 Elsevier B.V. All rights reserved.

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