

6th International Conference and Exhibition on

MATERIALS SCIENCE AND CHEMISTRY

May 17-18, 2018 | Rome, Italy

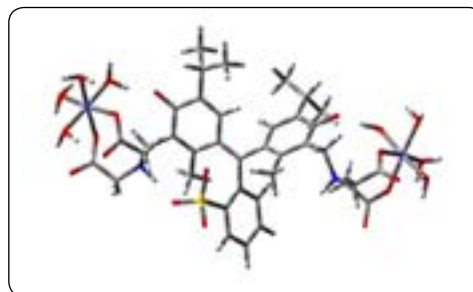
A joint spectrochemical, chemometrics and DFT/TD-DFT analysis of the Zn^{II}, Cu^{II} and Fe^{II} metal ions complexation by MTB in aqueous solution

Zolaikha Rasouli, Mehdi Irani, Sonia Jafari and Raouf Ghavami
University of Kurdistan, Iran

Over the past few years quantitative determinations of micro/macro minerals have attracted considerable attention. This attention is because of the essential role of minerals in various procedures i.e., medical, food, industrial and their numerous biological activities on human health. Chelation of chromomeric agents to metallic ions is one of the most efficient practices used in quantitative determination of micro/macro minerals in recent year. Herein, complexation systems formed by methylthymol blue (MTB) and Zn^{II}, Cu^{II} and Fe^{II} metal ions in an aqueous solution with pH=5.0 have been described from experimental and theoretical points of view. It was characterized using UV-Vis absorption spectroscopy combined with soft/hard chemometrics methods and time dependent density functional theory (DFT/TD-DFT) calculations. First, an exploratory analysis from the acid-base system of MTB and each of the complex formation systems was carried out by Marquardt-Levenberg, MCR-ALS and RAFA algorithms. The results revealed that Zn^{II} and Cu^{II} have the same behavior in confronting with MTB, both 1:2 and 1:1 stoichiometries of Zn^{II} or Cu^{II} to MTB. However, for Fe^{II}, simultaneous formation of FeL and Fe₂L complexes were suggested. In the second step of our work, we were interested to the description in detail of these systems by DFT/TD-DFT calculations to identify the nature of their structural geometries in the aqueous solution. For this purpose, we proposed the molecular hypothetical structures for different complex species based on the favorably moieties included in the complexation reactions, the protonation state of different functional groups of MTB and finally, the metal ion surrounding.

Recent Publications

1. S Supasai, L Aimo, A M Adamo, G G Mackenzie and P I Oteiza (2017) Zinc deficiency affects the STAT1/3 signaling pathways in part through redox-mediated mechanisms. *Redox Biology* 11:469-481.
2. K W Huang, C J Yu and W L Tseng (2010) Sensitivity enhancement in the colorimetric detection of lead(II) ion using gallic acid-capped gold nanoparticles: Improving size distribution and minimizing interparticle repulsion. *Biosensors and Bioelectronics* 25:984-989.
3. B Hemmateenejad, M Nekoeinia and G Absalan (2011) Spectrophotometric study of complex formation equilibria in the presence of interference using hard-soft net analyte signal method: Application to drug-metal complexation. *Analytica Chimica Acta* 683:178-186.
4. M Garrido, F X Rius and M S Larrechi (2008) Multivariate curve resolution-alternating least squares (MCR-ALS) applied to spectroscopic data from monitoring chemical reactions processes. *Analytica Chimica Acta* 390:2059-2066.
5. B Hemmateenejad, A Abbaspour, H Maghami and A Foroumadi (2008) Spectrophotometric determination of acidity constants by two-rank annihilation factor analysis. *Analytica Chimica Acta* 607:142-152.



Biography

Zolaikha Rasouli has obtained her Masters' degree in Science from Kurdistan University, UK in 2009. She was a PhD candidate in Analytical Chemistry, Kurdistan University, 2011. Her working field is focused on chemometrics modern methods at PhD level. She is currently working on a PhD thesis.

Rasouli_shahin@yahoo.com