Proceedings of the 3rd World Congress on Recent Advances in Nanotechnology (RAN'18)
Budapest, Hungary – April 10 - 12, 2018
Paper No. ICNMS 102
DOI: 10.11159/icnms18.102

Specific and Structural Study of Cu(II), Na(I) and CuNPs on Picolinic Acid Ligand

Sujittra Srisung[1], Nootcharin Wasukan[2], Mayuso Kuno[1]
[1]Department of Chemistry, Faculty of Science, Srinakharinwirot University
114 Sukhumwit 23, Wattana, Bangkok, Thailand
sujittras@g.swu.ac.th
[2]National Nanotechnology Center, National Science and Technology Development Agency
111 Thailand Science Park, Khlong Luang, Pathum Thani, Thailand

Extended Abstract

Nanotechnology is rapidly growing form of modern technology, which have been widely researched and the development of a drug [1-2]. Picolinic acid is interesting to the pharmaceutical industry because of interaction with metal ions in the body [3-5]. Copper nanoparticles (Cu NPs) are also used in consumer products which humans can exposed in their bodies [6-7]. In this study, the interactions between picolinic acid with copper (II), sodium (I) and CuNPs were studied by using the B3LYP/6-31G (d,p) method. The structures, position of the O-O bond and N-O bond, the binding energy of the complex ratios of picolinic acid to metal ions of copper (II) or sodium (I) in the ratio of 1 : 1 were investigated in this study. The result show that the picolinic acid and copper (II) at the position between N-O bond with the binding energy of -493.838 kcal/mol, which is found to be more stable than the position between O-O bond. However, the binding energy of picolinic acid and sodium (I) at the position between the O-O bond was estimated to be -155.501 kcal/mol and more stable than the position between N-O bonds due to the decreasing energy calculation. Therefore, copper (II) is more specific than sodium (I) with picolinic acid. In addition, the comparison specificity between picolinic with copper (II) and copper nanoparticles. The result show that the picolinic acid and copper nanoparticles at the position between N-O bond, found to be more stable than the position between O-O bonds with the binding energy of -5850.242 kcal/mol. Due to the fact that CuNPs are smaller than copper (II) and show the best specificity and ability to bind the picolinic acid.

References

[1] AF. Tuyun and H. Uslu, "Extraction equilibria of picolinic acid from aqueous solution by tridodecylamine (TDA)," *Desalination*, vol. 268, pp. 134-140, 2011.
[2] H. Tomioka, T. Shimizu, Y.Tatano, "Effects of picolinic acid on the antimicrobial functions of host macrophages against *Mycobacterium avium* complex," *Int J Antimicrob Agents*, vol. 29, pp. 460-464, 2007.
[3] R. S. Grant, S. E.Coggan, G. A. Smythe, "The Physiological action of picolinic acid in the human brain," *Tryp.Res*., vol. 2, pp.71-79, 2009.
[4] P. Koczon, J. Cz. Dobrowolski, W. Lewandowski, A. P. Mazurek, "Experimental and theoretical IR and Raman spectra of picolinic, nicotinic and isonicotinic acids," *J Mol Struct*, vol. 655, pp. 89-95, 2003.
[5] A. Cioczek-Czuczwar, P. Czuczwar, W. A. Turski, J. Parada-Turska, "Influence of picolinic acid on seizure susceptibility in mice," *Pharmacol Rep*., vol. 69, pp. 77-80, 2017.
[6] L. F. Wang, N. Habibul, D. Q. He, W. W. Li, X. Zhang, H. Jiang, H. Q. Yu, "Copper release from copper nanoparticles in the presence of natural organic matter, " *Water Research*, vol. 68, pp. 12-23, 2015.
[7] J. Robert, T. Griffit, W. Roxana, A. H. Kelly, D. D. Nancy, P. Kevin, T. David, S. B. David, "Exposure to copper nanoparticles causes gill injury and acute lethality in zebrafish (Daniorerio)," *Environ Sci Technol*, vol. 41, pp. 8178-818, 2007.