

Accepted Manuscript

Original article

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PII: S1319-6103(17)30054-6

DOI: <http://dx.doi.org/10.1016/j.jscs.2017.04.003>

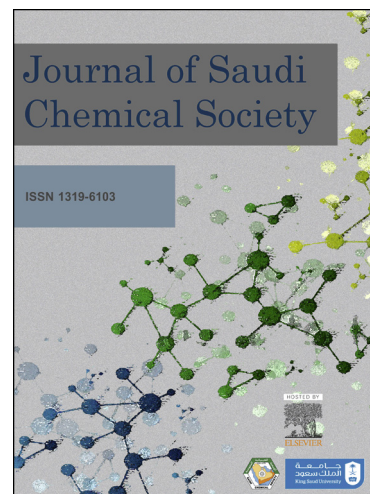
Reference: JSCS 870

To appear in: *Journal of Saudi Chemical Society*

Received Date: 1 February 2017

Revised Date: 27 March 2017

Accepted Date: 11 April 2017



Please cite this article as: A. Üngördü, N. Tezer, DFT study on metal-mediated uracil base pair complexes, *Journal of Saudi Chemical Society* (2017), doi: <http://dx.doi.org/10.1016/j.jscs.2017.04.003>

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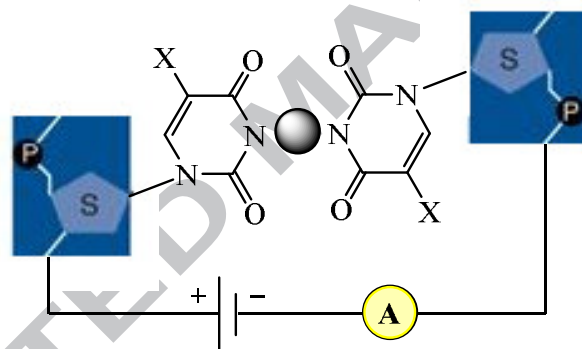
DFT study on metal-mediated uracil base pair complexes

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Cumhuriyet University, Faculty of Science, Department of Chemistry, 58140,
Sivas/TURKEY**Abstract**

The most stable of metal-mediated uracil base pair complexes were determined. Method was used density functional theory, B3LYP. The calculations of systems containing C, H, N, O were described by 6-311++G(d,p) and cc-PVTZ basis sets and LANL2DZ and SDD basis sets was used for transition metals. Then E_{gap} values of complexes were calculated and the electrical conductivity of the complexes for single nanowires were studied by band theory. Metal-mediated uracil base pair complexes which will used as conductive wires in nanotechnology were predicted. In nanoworld, this study is expected to show a way for practical applications.



Keywords electrical conductivity, metal-DNA, uracil, nanowires, DFT.

1. Introduction

Recently, DNAs and their derivatives have attracted much interest for the possibility of using such molecules as building blocks for electronic nano-devices (Scheme 1) [1-4]. Among these derivatives, metal-DNAs are obtained by treatment of DNA to metal ions [5]. Alkali (or rare-earth) ions form only electrostatic interactions with the nucleobases [6,7], but transition metal ions are expected to interact with the nucleobases also by chemical bonding [8-13]. However, transition metals are good carriers of many function particularly in the nanoworld. Therefore, they are also utilized for functionalization of DNA [14] among various modification schemes.

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