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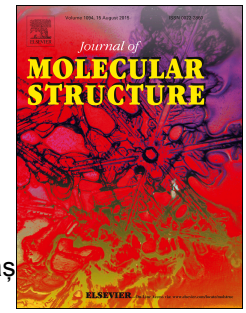

Investigations of structural, spectral, electronic and biological properties of N-heterocyclic carbene Ag(I) and Pd(II) complexes

Koray Sayin, Sultan Erkan Kariper, Merve Taştan, Tuba Alagöz Sayin, Duran Karakaş

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Investigations of Structural, Spectral, Electronic and Biological Properties of N-Heterocyclic Carbene Ag(I) and Pd(II) Complexes

Koray SAYIN*, Sultan ERKAN KARİPER, Merve TAŞTAN, Tuba ALAGÖZ SAYIN, Duran KARAKAŞ

krysayin@gmail.com and ksayin@cumhuriyet.edu.tr

Sivas Cumhuriyet University, Faculty of Science, Department of Chemistry, 58140 Sivas, Turkey

ABSTRACT

Computational analyses of two Ag(I) and two Pd(II) complexes were done. Benchmark analyses were performed to obtain the most appropriate calculation level for studied complexes. HF, B3LYP and M062X method were selected as calculation method. As for the basis set, lanl2dz, 6-31G, 6-31G(d) and 6-31G(d,p) were selected. LANL2DZ was used for metal atoms and the others were for the rest atoms in related molecules. The most appropriate calcualtion level was determined as B3LYP/6-31G(d)(LANL2DZ). Structural and spectral analyses (IR, UV-VIS and NMR) were performed. Additionally, non-linear optical (NLO) properties and biological properties were investigated and examined in detail. According to calculation results, complex (4) was found as the best candidate for NLO applications. Additionally, complex (4) was found as the best candidate for lung cancer drug.

Keywords: N-Heterocyclic carbene, Metal Complexes, NLO Properties, Molecular Docking, Computational Analyses

1. Introduction

N-heterocyclic carbene (NHC) complexes have significance properties in the inorganic and bio-inorganic chemistry. Recently, importance of their transition metal complexes is increasing day by day due to their biology, pharmacology and catalysis properties [1,2]. Palladium and platin complexes are especially considerable properties in the catalysis and polymerizations [3,4]. Due to the structural and electronic properties, copper, silver and gold complexes are major in the anti-cancer research. According to published paper, silver complex or compounds have antimicrobial, anti-fungal, anti-bacterial and anti-cancer properties [5-9].

In the last decade, computational research has attracted many researchers and academic journals. Such research has increased considerably and many articles have been published [10-15]. However, it should not be forgotten that computational chemistry has a light-tracing property to the experimental one.

In this paper, two Ag(I) and two Pd(II) N-heterocyclic carbene complexes are investigated. Related Ag(I) and Pd(II) complexes have been synthesized by Ghdhayeb et al. in 2017 [16]. X-Ray structures has been reported for just complex 2 [16]. Additionally, their biological properties against HCT116 cell have been reported in their paper. Two dimensional (2D) structures are represented in Schema 1.