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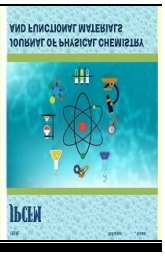

Investigation of Hartree-Fock and Density Functional Theory of Platinum(II) Complex

[a,*] *Hunar Hama KHALID,* [b] *Sultan ERKAN,* [a] *Niyazi BULUT*

[a] *Department of Physics, Faculty of Science, Firat University, 23169 Elazig Turkey*

[b] *Department of Chemistry and Chemical Processing Technologies Cumhuriyet University Yildizeli Vocational School 58140 Sivas, Turkey*

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ABSTRACT

In this study, we investigate both hatree-fock and density functional theory of platinum complex in detail. Hence, before quantum mechanical calculations were optimized using various methods and basis sets. For appropriate calculation level, according to the correlation between the calculated and experimental, we found out at M062X / CEP-31G for our platinum(II)complex. Finally, we have compared all our result with the data available in the literature.

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Density functional theory
Platinum (II) complex
Correlation determination

1. Introduction

The research of Pt(II) complexes with amino acids is quite successful both because of their biological activity and because of their use in solving basic issues in the coordination of geometrical complexes with multifunctional [1]. It was found that showed significantly higher cytotoxicity to human lung cancer cells and human prostate cancer cells RV1 [2].

Functional density theory is a mechanical quantity technique used in physics and chemistry to explore and quantify the physical characteristics of atoms, molecules, and solids [3]. The recent impact of density functional theory (DFT) on quantum chemistry progression is significant and could be attached to the achievement of so-called "chemical accuracy" at the end of the 1980s while gradient-corrected and hybrid functional methods were implemented [4].

The theory of Hartree-Fock is essential to the most theory of electronic structures. It is the foundation of the concept of molecular orbital (MO) that suggests that the movement of each electron can be characterized by a single-particle (orbital) feature that does not rely explicitly on the other electrons ' instantaneous movements. The theory of Hartree-Fock often offers a great starting point for more elaborate theoretical techniques that are better estimated to the electronic equation of Schrodinger [5]. The Hartree – Fock technique is commonly used for estimated computations of the electronic structure in quantum chemistry. The theory of Hartree – Fock is a variation of this problem of minimization [6].

2. Computational details

2.1. Synthesis

Pt(dpb)I was produced as the following procedure. Acetonitrile solution 30 mL containing Pt(dpb)Cl 50 mg(0.1 mmol) was stirred for 20 min. AgOTf (51.3 mg 0.2 mol) dissolved in a small amount of acetone was added to the solution. After the stirring for 40 min, tetrabutylammonium iodide (TBAI) 886 mg (2.4 mmol) was added little by little. Further stirring for 2 h and subsequent removal of solvent gave a yellow-white powder. Purification of the material by silica-gel column chromatography with $CHCl_3$ as an eluent and recrystallization from CH_2Cl_2–hexane provided a yellow powder. Pt(dpb)I: ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.48(t, H), 7.38t, H), 7.71(d, H), 8.05(d, H), 8.18(t, H), 9.83(d, H) [7].

* Corresponding author:
E-mail (hunaranwar26@gmail.com)

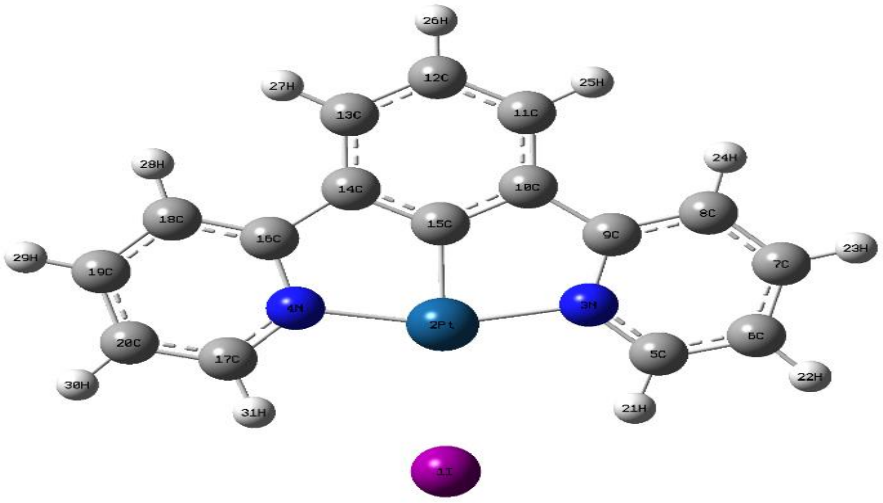

Figure 1. The symbolic optimized structure of Pt(dpb)I.

Table 1. Coefficient of determination.

		CEP-4G	CEP-31G	CEP-121G	Lanl2dz	Lanl2mb	SDD
M062X	R^2	0.7701	0.9520	0.9206	0.8928	0.8923	0.9028
B3LYP	R^2	0.8197	0.8538	0.8125	0.4877	0.8918	0.8525
HF	R^2	0.3821	0.6038	0.6224	0.7032	0.7569	0.7080

2.2. Method

The input files of relevant complexes were prepared with GaussView 5.8. All other calculations were performed with Gaussian 09 using B3LYP and M062X methods by density functional and Hartree-Fock calculation. DFT and HF calculations were carried out using B3LYP and M062X methods and CEP-4G, CEP-31G, CEP-12G, LanL2DZ, LanL2MB, and CDD basis sets. The geometry was fully optimized in the ground states.

3. Results and discussion

The coefficient of determination (R^2) between the experimental and measured variables is calculated in Table 1. It provides the ratio of the variance between one variable and the other. Coefficient of determination can be discovered in the spread diagram R^2. When considering R^2 values, R^2 is closer to 1 at M062X / CEP-31G level.

Then the complex was optimized with the DFT-M062X method and CEP-31G. Figure (1) displays the symbolic optimized structure of Pt(dpb)I.

We investigated both HF and DTF calculation for Pt(dpb)I with the mentioned basis sets. By applied correlation determination; we got some result that showed in table 1. The table demonstrates HF calculation farther to one compare to DFT calculation, which the basis sets CEP-4G, CEP-31G, CEP-121G, Lanl2DZ, SDD and Lanl2MB were arranged respectively. In the case of DFT, we investigated B3LYP and M062X methods. We found out M062X closer to one than B3YLP, especially at M062X/CEP-31G closer at one compare the rest of them.

4. Conclusion

In this study, we investigated both HF and DTF calculation, which we display DFT is better and more accurate than HF. We demonstrate that B3YLP farther to one than M062X in general. In a case carrying out of HF, we displayed Lanl2MB closer at one while CEP-4G is farther. As well as in a case using B3YLP, Lanl2MB is closer to one and Lanl2DZ is farther.

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