Journal of Engineering and Applied Sciences 14 (Special Issue 7): 9936-9945, 2019
ISSN: 1816-949X

Optimized Structure Investigation of Platinum Complex (VI) using DFT

Lekaa Hussain Khdaim and Abbas Abd-Ali Draea
Department of Chemistry, College of Science, University of Babylon, 51002 Hillah, Babylon, Iraq

Abstract: Optimized structure investigation of (bis (methoxyamino) bis ((methoxycarbamoyl) oxy) platinum (VI) chloride) (MMP chloride) has been achieved using DFT at B3LYP/Lanl2DZ level of theory. Gaussian packaged program G09 has been used with the relationship between their molecular and electronic structure of platinum complex (VI). The electronic properties such as HOMO, LUMO, Egap, thermodynamic properties such as ΔG, ΔH, ΔS and global reactivity descriptors such as hardness, softness, ionization potential, electron affinity, electro gravity, chemical potential, electro philicity and electronic charge were calculated for Pt (VI) complex. Reactivity of the MMP chloride is always governed but its electronic properties and kinetic and thermodynamic stability. Theoretical spectrograms for the IR and NMR spectrum were also constructed in RHF but UV spectrum in UHF at B3LYP levels. They found the symmetry of Pt (VI) complex form is C1 refer to asymmetrical distribution in the Pt (VI) complex. Large values of the energy gap of platinum complex (VI) that's imply high electronic stability and then low reactivity when low values imply that it will be easy to remove an electron from HOMO orbital to LUMO as indication of reactivity. Thermodynamic calculation of complex A by using DFT/B3Lyp/LanL2DZ which is endothermic and nonspontaneous (195.8446, 135.7806 kCal/MoL) and energy gap is 0.07754 kCal/mol. The stabilized structure of MMP chloride comes out by total energy which equal to -1209.074 a.u.

Key words: Optimized structure, DFT, MMP chloride, B3LYP, theoretical spectra, stabilized

INTRODUCTION

Anticancer activity of cisplatin complexes have been discovered great deal attention, since, drawn to platinum compound of Pt (II) and Pt (VI) (Burda and Leszczynski, 2003). Pt (II) and MMP chlorides are widely used compounds with cytotoxic activity. Pt (II) complexes readily react with DNA to form intrastrand cross links (Pinto and Lippard, 1985). Cisplatin has been widely used in medicine with regard to its antitumor properties including the treatment of various solid tumors (Dolezel and Kuban, 2002). Platinum drugs are used for treatment of specific cancer, testicular, ovarian, bladder, head and neck, esophageal small or non-small cell lung breast cervical, stomach and prostate cancers (Abu-Surrah and Kettunen, 2006). Side effects of platinum therapy include general cell damaging effects, vomiting, nausea, decreased blood cell and platelet production in bone marrow and decreased response to infection (Boyiadzis, 2007; Kelland, 2007; Ko *et al*., 2008). Platinum (II) complex in the main or side chains have attached much attention because of their unique electronic properties. Internal charge transfer from an electron rich unit to an electron deficient unit has been extensively used to obtain the low band gap of the molecules (Fitri *et al*., 2014; Sadiki *et al*., 2014; Belghiti *et al*., 2014). Also platinum group elements can be naturally found only at very low concentration (Sikorova *et al*., 2011). Platinum compounds are still the most effective cytostatic drugs such as Ru (II), Os (II), Ir (II) have quite similar properties (Dhahagani *et al*., 2014). Equation of the leaving groups chloride for cisplatin, carboxylate for carboplatin, generates reactive cisplatin which cisplatin react readily with purine nucleobase in DNA (Wilson and Lippard, 2011). The stable of MMP chloride their low spin d^6 electronic configuration, aids in their survival of the acidic environment of the stomach before being absorbed to the blood stream (Wilson and Lippard, 2011). Approaches to finding such agents often depend on novel design strategies employ bioactive vectors such as intercalates, amino acid, sugars, bile acids, folates and estrogen analogues (Ho *et al*., 2003).

MATERIALS AND METHODS

Experimental details: The optimized geometry been done in the vibrational frequency calculation at the RHF through DFT method to characterize all stationary points as minima (Fig. 1). The vibrational frequency assignments were made with a high degree of accuracy with the help Gaussain 98 suite of program (Frisch *et al*., 2010).

Corresponding Author: Lekaa Hussain Khdaim, Department of Chemistry, College of Science, University of Babylon, 51002 Hillah, Babylon, Iraq

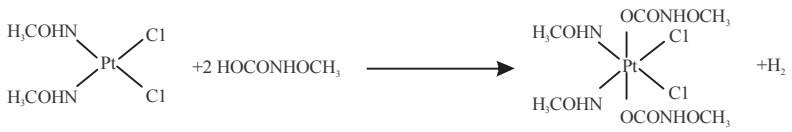


Fig. 1: (VI) complex from cisplatin in gas phase (Wilson and Lippard, 2011)

The H^1, C^{13} chemical shifts of bis (methoxyamino) bis ((methoxycarbamoyl) oxy) platinum (VI) chloride (MMP chloride) was calculated using RHF and DFT calculation with LanL2DZ basis set but UHF which using UV spectra was calculated. The HOMO and LUMO were studied to calculate the energy gap (E) (Adnan *et al*., 2014; Abbas and Nadia, 2012). Thermodynamic parameters were calculated by DFT method B3LYP at level of theory level. The B3LYP, aversion of the DFT method using Becke's three parameter functional (B3) and including a mixture Hartree-fock with DFT exchange terms associated with the gradient corrected correlation functional of Lee, Yang, Parr (LYP (Adnan *et al*., 2014).

RESULTS AND DISCUSSION

Structural and electronic properties have been calculated and can be discuses as follow:

Eometry optimization: Figure 2 represented the optimized structure of Pt (VI) complex they found some of selected mean bounds of complexes such as bond lengths in the MMP chloride and bond angle and dihedral angle of complex in the ground state in Table 1.

The bond length between Pt atom and O, N, Cl atoms are very important in the load transfer charge between donor and acceptor group in the compound, it the bond length favors in the intramolecular charge transfer when is shorter.

Thermodynamic

Properties: Thermodynamic properties were calculated using DFT and were obtained from the output of Gaussian programs. The stability of a molecular structure is determined o f total energy of the molecule is low. The ZPE is the lowest possible energy that quantum mechanical system can have. The enthalpy values for bis (methoxyamino) bis ((methoxycarbamoyl) oxy) platinum (VI) chloride (MMP chloride) is not meaningful rather bond dissociated energy are considered better description of stability of the compound and entropy value is not random but Gibbs free energy is non spontaneous for bis (methoxyamino) bis ((methoxycarbamoyl) oxy) platinum (VI) chloride (MMP chloride) in Table 2.

Energy levels: The energy of the frontal molecular orbital such as EHOMO, ELUMO and Egap for MMP chloride were calculated by the DFT with B3LYP/Lanl2DZ. The energy of EHOMO is often associated with the electron donating ability of the molecules whereas the energy of ELUMO is associated with the electron accepting ability of the molecules (Abbas and Nadia, 2012). The high value of the EHOMO indicates a high tendency to donate electrons to suitable acceptor molecule with low empty molecular orbital energy also the value of the LUMO indicate a high tendency to accept electrons from the metal. The results given in Table 3, show which the bis (methoxyamino) bis ((methoxycarbamoyl) oxy) platinum (VI) chloride (MMP chloride) has the higher energy of HOMO. The energy gap between the HOMO and LUMO energy levels of MMP chloride (Khalil *et al*., 2013). Large values of the energy gap imply high electronic stability and then low reactivity when low values imply that it will be easy to remove an electron from HOMO orbital to LUMO which can be good result in reactivity. The electronic dipole moment which measure of bond properties also indicate higher dipole moment (6.337 Debye) (Bourass *et al*., 2015) (Fig. 3 and 4).

Global reactivity: Global reactivity description were shown into Table 4, it was possible to calculate the energy value of the electronic affinity, ionization potential, electronegativity, hardness, softness, electrophilicity and chemical potential (Khudhair *et al*., 2017). The electronegativity is the chemical properties that ability of molecule to attract electrons towards itself in a covalent bond. Also according to sanderson's electronegativity equalization principle, also the value is lowest in the gas phase this behavior indicate of bis (methoxyamino) bis ((methoxycarbamoyl) oxy) platinum (VI) chloride (MMP chloride), the hardness and softness is important propertiesto measure the molecular stability and reactivity the small energy gap is soft molecule (Mendoza-Huizar, 2014). The number of electron transferred (N). If $N<3.6$ the stability of MMP chloride increasing by increasing electron donating ability of these complex moreover, the value of w is measure the susceptibility of chemical species to accept electron thus, low values of w due to a good neocleophilies (Mendoza-Huizar, 2014) (Table 5 and 6).

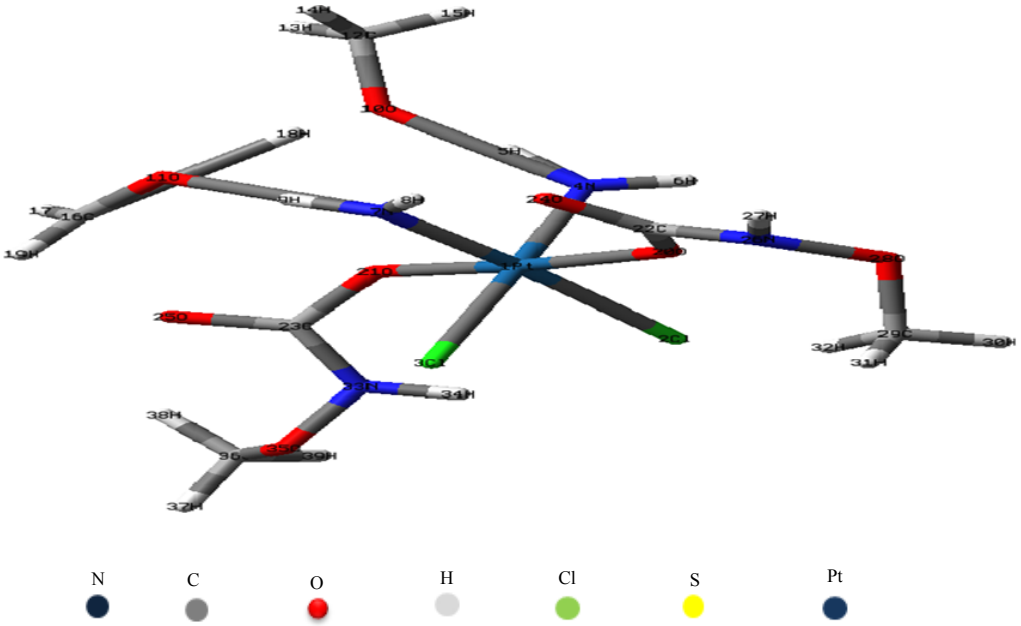


Fig. 2: Geometry optimized structure of bis (methoxyamino) bis ((methoxycarbamoyl) oxy) platinum (VI) chloride (MMP chloride) by DFT/B3Lyp/LanL2DZ (5 D, 7 F) at level of theory

Table 1: Name and molecule structure of MMP chloride

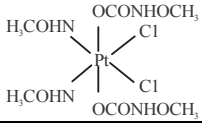
Abbreviation	Structure	IUPAC name
MMP chloride		Bis (methoxyamino) bis ((methoxycarbamoyl) oxy) platinum (VI) chloride

Table 2: Theoretical parameter of bond length and bond angle bis (methoxyamino) bis ((methoxycarbamoyl) oxy) platinum (VI) chloride (MMP chloride) by using DFT/B3Lyp/LanL2DZ at level of theory

Bond types	Length bond (nm)	Angle type	Bond angle (Å)	Dihedral types	Dihedral
Pt_1-N_4	1.98	Pt_1-N_4-O_{10}	90.0	Cl_{17}-O_{16}-Pt_1-Cl_2	180
Pt_1-Cl_2	2.29	Pt_1-O_{10}-C_{11}	120	O_5-N_4-Pt_1-Cl_2	-90
Pt_1-O_{10}	1.94	Cl_{17}-O_{16}-Pt_1	120	C_6-O_5N_4-Pt_1	180
Cl_{17}-O_{16}	1.34	O_5-N_4-Pt_1	120		
O_5-N_4	1.32	N_7-Pt_1-N_4	82.2		
C_6-O_5	1.40	C_6-O_5N_4	1.20		

Table 3: Thermodynamic calculation of bis (methoxyamino) bis ((methoxycarbamoyl) oxy) platinum (VI) chloride (MMP chloride) by using DFT/B3Lyp/Lan2DZ at 298.150 K at levels of theory

Functions	ΔH kcalmol^{-1}	ΔG kcalmol^{-1}	ΔS calmol^{-1}	ZPE kcalmol^{-1}	Imaginary frequencies	Total energy-E (a.u)	Degree of freedom	Full point group
MMP chloride	195.8446	135.7806	201.4556	169.4268	+	1209.074	111	C1

Table 4: Energy levels for bis (methoxyamino) bis ((methoxycarbamoyl) oxy) platinum (VI) chloride (MMP chloride) at DFT/B3LYP/LanL2DZ (5 D, 7 F) at levels of theory

Functions	ELUMO (kcalmol^{-1})	EHOMO (kcalmol^{-1})	ΔE gap (kcalmol^{-1})	Dipole moment (D)
MMP chloride	0.01665	-0.06104	0.07754	6.337

Table 5: Physical properties for bis (methoxyamino) bis ((methoxycarbamoyl) oxy) platinum (VI) chloride (MMP chloride) at DFT/B3LYP/LanL2DZ (5 D,7 F) at levels of theory

Physical properties	Ionization Potential (IP)	Electron Affinity (EA)	Electronegativity (X)	Absolute hardness (η)	Chemical Softness (S)	Chemical Potential (π)	Absolute softness (σ)	Global electrophilicity (ω)	Additional electronic charge (ΔN)
Values	0.0610 kJmol^{-1}	-0.0167 kJmol^{-1}	-0.0395 eV	-0.0777 eV	-6.50 eV	0.0395 eV	-12.87	-9.811×10^{-3}	0.5

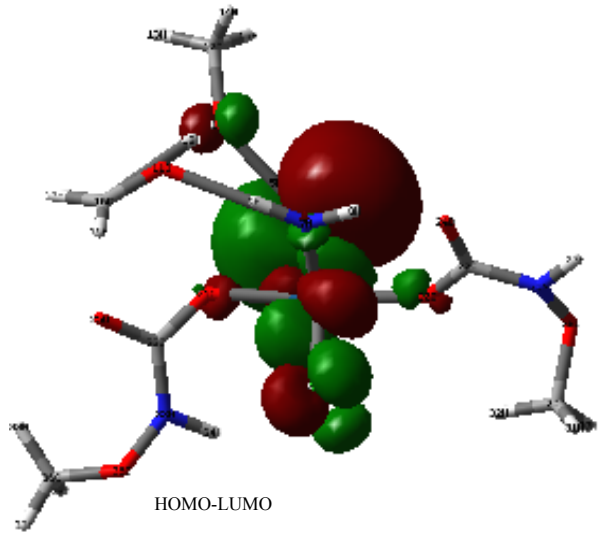


Fig. 3: Frontial molecular orbital's of 3D for bis (methoxyamino) bis ((methoxycarbamoyl) oxy) platinum (VI) chloride (MMP chloride) by DFT/ B3Lyp/LanL2DZ (5 D, 7 F) at level of theory

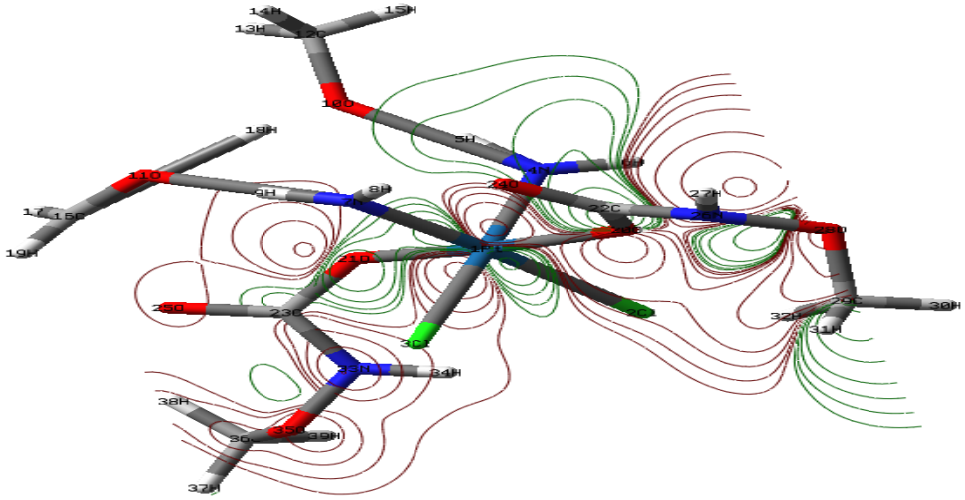


Fig. 4: Frontal molecular orbital of 2D for bis (methoxyamino) bis ((methoxycarbamoyl) oxy) platinum (VI) chloride (MMP chloride) by DFT/B3Lyp/LanL2DZ (5 D, 7 F) at level of theory

Table 6: Energies value of chemical reaction of bis (methoxyamino) bis ((methoxycarbamoyl) oxy) platinum (VI) chloride (MMP chloride) by DFT/B3Lyp/LanL2DZ (5d,7f) at level of theory

Chemical species	Total energy	IR freq.	ZPE kCal.mol^{-1}	ΔH kCal.mol^{-1}	ΔG kCal.mol^{-1}	ΔS Cal.mol^{-1}
$PtCl_4$	178.039	-	2.7410	7.241	-16.9200	81.040
$2NH_3$	111.740	+	43.4800	50.060	22.6400	91.960
$PtCl_4(NH_3)_2$	292.280	-	46.2500	58.030	19.5500	129.060
$PtCl_2(NH_3)_2$	262.290	+	49.8500	57.980	29.6500	95.020
Cl_2	918.870	+	0.7040	2.941	-13.0500	53.630
CH3OCl	574.404	-	29.0273	34.224	5.8345	95.219
$PtCl_2(NH_2OCH_3)_2$	491.197	+	88.1163	100.732	63.8640	123.655
H_2O_2	150.690	-	16.2800	19.330	3.0600	54.580
$PtCl_2(NH_2OCH_3)_2(OH)_2$	642.059	+	103.3680	119.131	76.4230	143.243
$2HOCONHOCH_3$	358.480	+	57.3190	66.126	33.1160	110.716
$PtCl_2(NH_2OCH_3)_2(OCONHOCH_3)_2$	1209.080	+	169.9200	195.843	135.7910	201.420
$2H_2O$	75.580	+	26.2500	32.000	5.1700	89.980

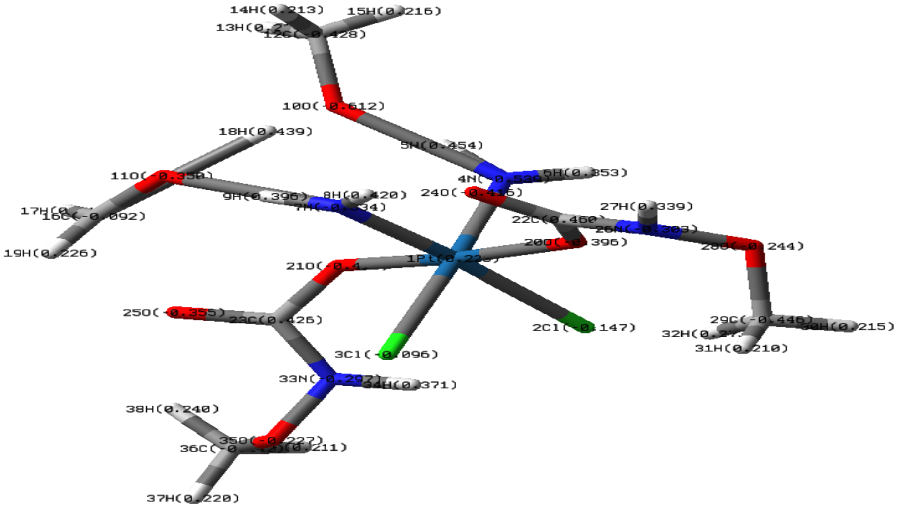


Fig. 5: Mullikan chargefor bis (methoxyamino) bis ((methoxycarbamoyl) oxy) platinum (VI) chloride (MMP chloride) by DFT/B3Lyp/LanL2DZ (5 D, 7 F) at level of theory

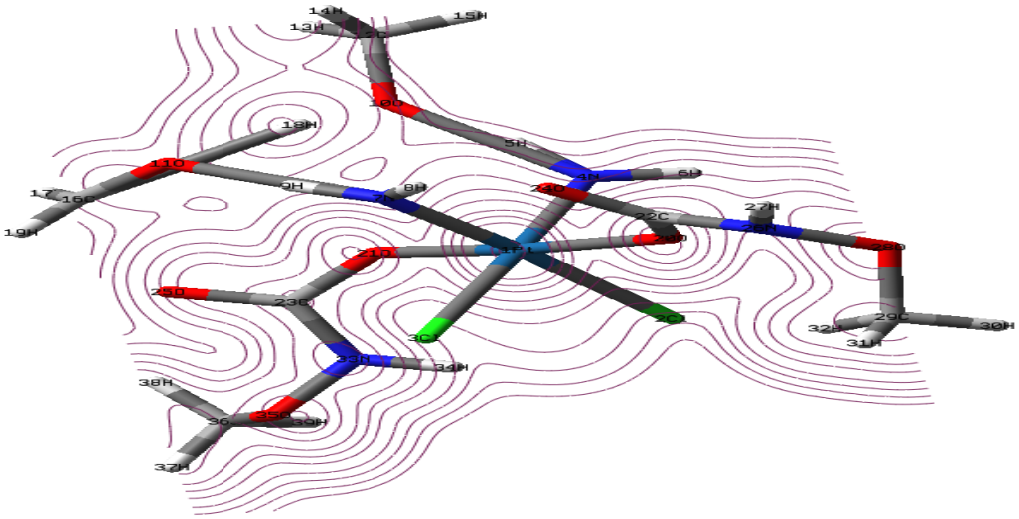


Fig. 6: Total density of 2D for bis (methoxyamino) bis ((methoxycarbamoyl) oxy) platinum (VI) chloride (MMP chloride) by DFT/B3Lyp/LanL2DZ (5 D, 7 F) at level of theory

The electron density is typically showed a comparison of the identified electron density with that predictable by spherical models of the atoms and is called distortion electron density. The negative charge are remarked by red color are distribution on the oxygen atoms in carbonyl groups and the nitrogen in amine group due to high value of electronegativity (Obi-Eghedi *et al*., 2011). The positive charge are remarked by green color are distribution on carboneatoms (Kooh *et al*., 2014). The Mullikan atomic charges give a positive value for C and H and negative values for O, N, Cl atoms. Figure 5-7 represent of Mullikan charge electron density and ESP, respectively (Adnan *et al*., 2014).

Reaction of $PtCl_4$ with NH_3: The chemical reaction of $PtCl_4$ with NH_3 can be occurs through multistep to give final product to obtained the net equation of reaction. Table 6 and Scheme 1 shows the total energies values of chemical species that's participating in the reaction. The net equation consisted from one mole of $PtCl_4$ with two mole of NH_3. The reaction is exothermic ΔH_{net} = -19.311571 kCal.mol^{-1}.

According to rate constant values, the rate determining step have been suggested depending on the steady state approximation. Scheme 1, represent the determination of effective concentration on the reaction rate can be derived of reaction rate law for the reaction mechanism according to the steady state approximation, the net rate of change equal zero for intermediates (Izet *et al*., 2012):

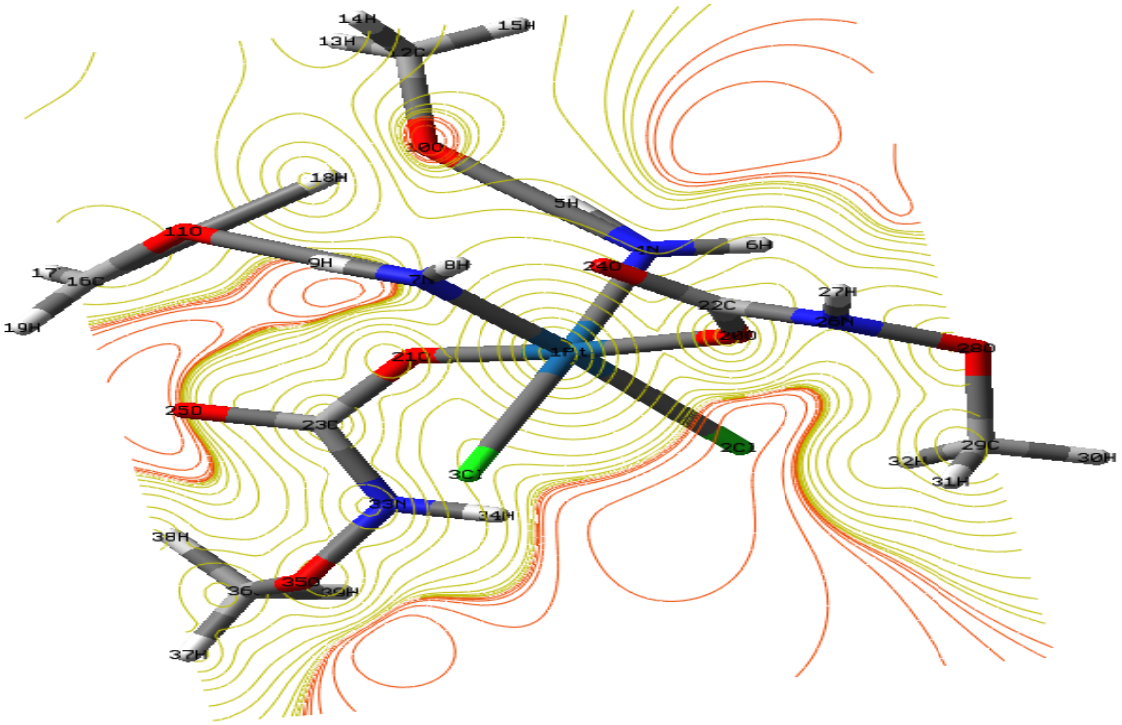


Fig. 7: Energy surface potential of 2D for bis (methoxyamino) bis ((methoxycarbamoyl) oxy) platinum (VI) chloride (MMP chloride) by DFT/B3Lyp/LanL2DZ (5 D, 7 F) at level of theory

$$PtCl_4+2NH_3 \underset{\grave{k}_1}{\overset{k_1}{\rightleftharpoons}} PtCl_4(NH_3)_2 \quad (1) \qquad \begin{aligned} Rate &= k_1[PtCl_4][NH_3]^2 \\ &= \grave{k}_1[PtCl_4(NH_3)_2]] \end{aligned}$$

$$PtCl_4(NH_3)_2 \underset{\grave{k}_2}{\overset{k_2}{\rightleftharpoons}} PtCl_2(NH_3)_2+Cl_2 \quad (2) \qquad \begin{aligned} Rate &= k_2[PtCl_4(NH_3)_2] \\ &= \grave{k}_2[PtCl_2(NH_3)_2][Cl_2] \end{aligned}$$

$$Pt(NH_3)_2Cl_2+2CH_3COCl \underset{\grave{k}_3}{\overset{k_3}{\rightleftharpoons}} Pt(NH_2OCH_3)_2Cl_2+2HCl \quad (3) \qquad \begin{aligned} Rate &= k_3[PtCl_2(NH_3)_2][CH_3COCl]^2 \\ &= \grave{k}_3[PtCl_2(NH_2OCH_3)_2](HCl)] \end{aligned}$$

$$Pt(NH_2OCH_3)2Cl_2+H_2O_2 \underset{\grave{k}_4}{\overset{k_4}{\rightleftharpoons}} Pt(NH_2OCH_3)_2Cl_2(OH)_2 \quad (4) \qquad \begin{aligned} Rate &= k_4[PtCl_2(NH_2OCH_3)_2][H_2O_2] \\ &= \grave{k}_4[[PtCl_2(NH_2OCH_3)_2(OH)_2 \end{aligned}$$

$$Pt(NH_2OCH_3)_2Cl_2(OH)_2+2HOCONHOCH_3 \underset{\grave{k}_5}{\overset{k_5}{\rightleftharpoons}} Pt(NH_2OCH_3)_2Cl_2(OCONHOCH_3)_2+2H_2O \quad (5)$$

$$\begin{aligned} Rate &= k_5[PtCl_2(NH_2OCH_3)_2(OH)_2][HOCONHOCH_3]^2 \\ &= \grave{k}_5[[PtCl_2(NH_2OCH_3)_2(OCONHCOCH_3)_2[H_2O]^2 \end{aligned}$$

Reaction rate law of BBMP as shown:

$$\frac{d[PtCl_4](NH_3)_2}{dt} = k_1[PtCl_4][NH_3]_2\text{-}\grave{k}_1[PtCl_4(NH_3)_2]\text{-}k_2[PtCl_4(NH_3)_2]+\grave{k}_2[PtCl_2(NH_3)_2][Cl_2] = 0 \quad (6)$$

$$\frac{d[PtCl_2(NH_3)_2]}{dt} = k_2[PtCl_2][NH_3]_2\text{-}\grave{k}_2[PtCl_4(NH_3)_2][Cl_2]+k_3[PtCl_2(NH_3)_2][CH_3COCl]^2+ \quad (7)$$
$$\grave{k}_3[PtCl_2(NH_2OCH_3)_2][HCl]^2 = 0$$

Therefore from Eq. 8-9 get on:

$$k_1[PtCl_4][NH_3]_2-\grave{k}_1[PtCl_4(NH_3)_2]-k_5[Pt(NH_2OCH_3)Cl_2(OH)_2][HOCONHOCH_3]+$$
$$\grave{k}_5[Pt(NH_2OCH_3)_2Cl_2(OCONHOCH_3)_2)][H_2O]^2 = 0$$

$$[PtCl_4(NH_3)_2] = \frac{k_1[PtCl_4][NH_3]_2-\grave{k}_5[Pt(NH_2OCH_3)_2Cl_2(OCONHOCH_3)_2]}{\grave{k}_1+k_5[Pt(NH_2OCH_3)Cl_2(OH)_2][HOCONHOCH_3]} \quad (10)$$

$$Rate = k_2[PtCl_4(NH_3)_2] \quad (11)$$

By substitution Eq. 10-11 get on:

$$Rate = k_3 \cdot \frac{k_1[PtCl_4][NH_3]_2+\grave{K}_5[Pt(NH_2OCH_3)_2Cl_2(OCONHOCH_3)_2]}{\grave{k}_1+K_5[Pt(NH_2OCH_3)Cl_2(OH)_2][HOCONHOCH_3]} \quad (12)$$

Equation (4-113) is consisted from two different probabilities: The first probability is to impose k_5 (6.09141×10^{12}> $\grave{k}_1$ (6.3508×10^{-12}), the equation will be as follow:

$$Rate = \frac{k_1[PtCl_4][NH_3]_2+\grave{K}_5[Pt(NH_2OCH_3)_2Cl_2(OCONHOCH_3)_2]}{K_5[Pt(NH_2OCH_3)Cl_2(OH)_2][HOCONHOCH_3]} \quad (13)$$

The secondary probability is to impose k_1 (6.3508×10^{-12})>k_5 (6.0914×10^{12}), the equation will be as follow:

$$Rate = \frac{k_1[PtCl_4][NH_3]_2+\grave{K}_5[Pt(NH_2OCH_3)_2Cl_2(OCONHOCH_3)_2]}{\grave{k}_1}$$

Scheme 1: The net equation of reaction $PtC1_4$ with NH_3 in vacuum

k_1 is very small and can be ignored, therefore, the predominant probability is k_5>k_1 and the rate determination step as follow in Eq. 1-13.

Vibrational band analysis: The position of the important bands of the Pt (VI) complex are shown Fig. 8. According to theoretical calculations of bis (methoxyamino) bis ((methoxycarbamoyl) oxy) platinum (VI) chloride (MMP chloride) energy structure belongs to the C1 point group symmetry. The scaling factors 0.964 for DFT and RHF values and the complex these band of the following: v (Pt-O) Asy = 369.17 cm^{-1}, v (Pt-Cl) Asy = 324.28 cm^{-1}, v (Pt-N) Asy = 552.65 cm^{-1}, v (C-O) Asy = 757.87 cm^{-1}, v (N-H) sym = 3546.39 cm^{-1}, v (N-O) Asym = 881.0 cm^{-1}, v (C-N) sym = 1392.31 cm^{-1}, v (C-H) sym = 3314.77 cm^{-1}.

Electronic properties: The model of electronic properties of bis (methoxyamino) bis ((methoxycarbamoyl) oxy) platinum (VI) chloride (MMP chloride) as seam in Fig. 9, display density of the electron clouds at different energy levels. The information related where the electron clouds are concentrated will be useful to predict whether the electron transfer electron system is efficient (Mendoza-Huizar, 2014). The result indicate lowest single electronic excitation is σ-σ* and n-σ*.

Chemical shift: Chemical shifts of 13C and 1 H-NMR in MMP chloride were investigated as shown in Fig. 10 (a, b). The chemical shifts of 13 C and 1 H-NMR in bis (methoxyamino) bis ((methoxycarbamoyl) oxy) platinum (VI) chloride (MMP chloride) as referred by TMS were separated around 28-192 and 1.75-12.5 ppm, respectively. This behavior was influenced by magnetic shielding effect on the bis (methoxyamino) bis ((methoxycarbamoyl) oxy) platinum (VI) chloride (MMP chloride). The separated chemical shifts of 13 C and 1 H-NMR were caused by nuclear spin interaction in carbon and proton atoms on bis (methoxyamino) bis ((methoxycarbamoyl) oxy) platinum (VI) chloride (MMP chloride). The chemical shift was mainly caused by hybridization of d spin in metal. The chemical shifts of 13 C and 1 H NMR MMP chloride depended on the electron density distribution with a slight deviation of charge density on bis (methoxyamino) bis ((methoxycarbamoyl) oxy) platinum (VI) chloride (MMP chloride) (Suzuki and Oku, 2016).

Significance: Molecular modeling of platinum complex (VI) (MMP chloride) by using DFT/B3LYP/LANL2DZ. Study of physical properties and Global reactivity. Also the synthesis of platinum (VI) complex from cisplatin in gas phase and the rate determining step have been suggested depending on the steady state approximation.

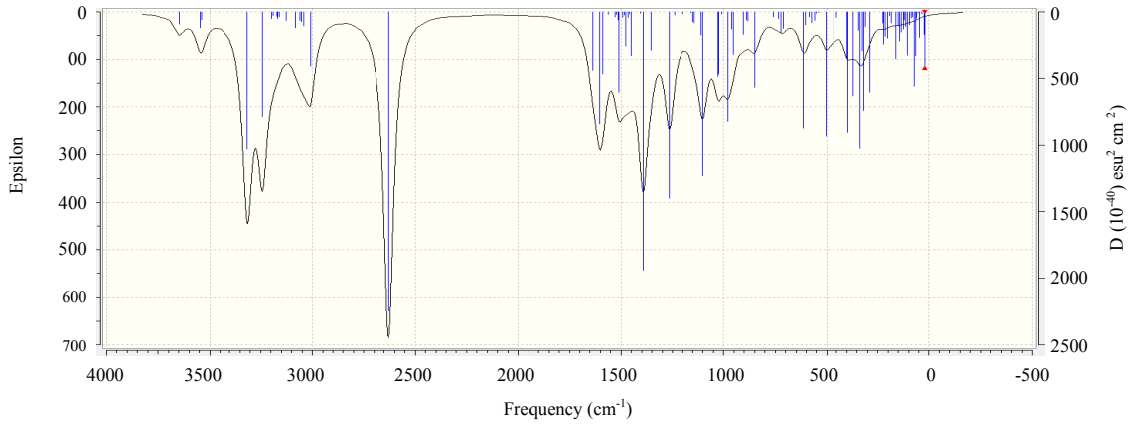


Fig. 8: Theoretical vibrational spectrum of bis (methoxyamino) bis ((methoxycarbamoyl) oxy) platinum (VI) chloride (MMP chloride) by DFT/B3Lyp/LanL2DZ (5 D, 7 F) at level of theory (IR spectrum)

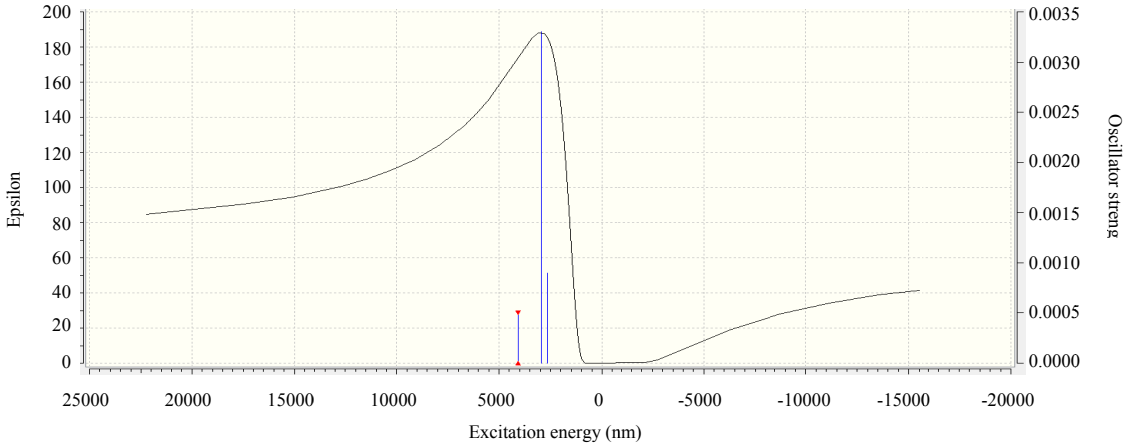


Fig. 9: Theoretical electronic transition spectrum of bis (methoxyamino) bis ((methoxycarbamoyl) oxy) platinum (VI) chloride (MMP chloride) by DFT/B3Lyp/LanL2DZ (5 D, 7 F) at level of theory (UV-VIS spectrum)

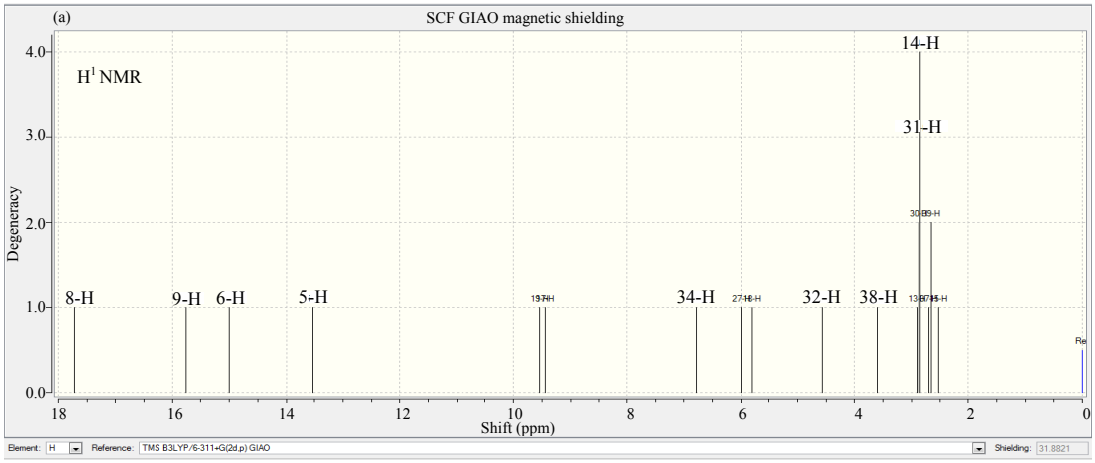


Fig. 10: Continue

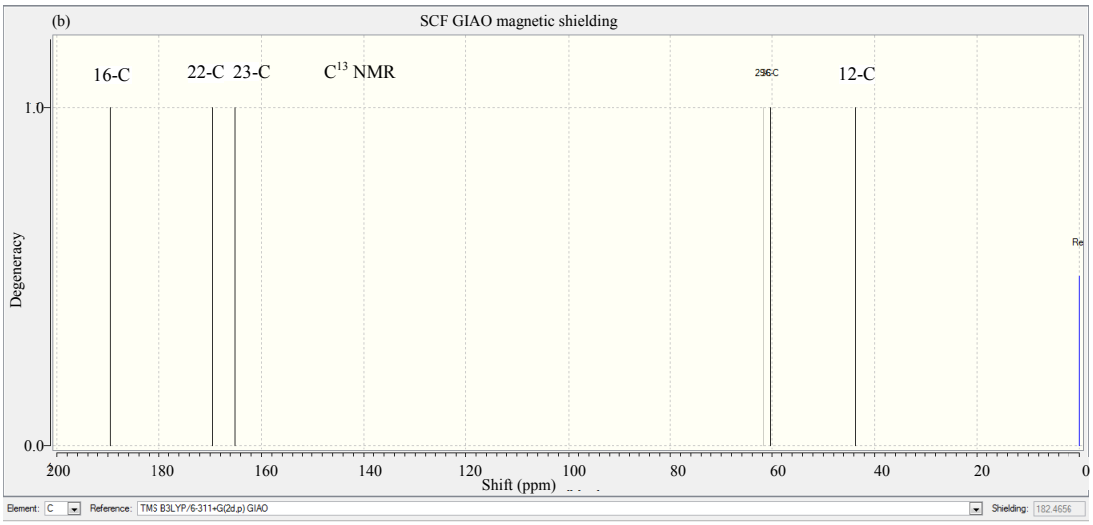


Fig. 10: Theoretical spectrum for bis (methoxyamino) bis ((methoxycarbamoyl) oxy) platinum (VI) chloride (MMP chloride) by DFT/B3Lyp/LanL2DZ (5 D, 7 F) at level of theory; a) H^1 NMR and C^{13} NMR

CONCLUSION

The geometry optimized structure of Pt (VI) complex have been calculated using DFT based on B3Lyp/LanL2DZ at level of theory in vacuumed. The symmetry of Pt (VI) complex form is C1 refer to asymmetrical distribution in the Pt (VI) complex. The output of this Pt (VI) complex gave C1 symmetry which is wrong symmetry.

Thermodynamic calculation of complex A by using DFT/B3Lyp/LanL2DZ which is endothermic and nonspontaneous 195.8446, 135.7806 $kCalmol^{-1}$ respectively and energy gap value is 0.07754 $kCalmol^{-1}$. The stabilized structure of bis (methoxyamino) bis ((methoxycarbamoyl) oxy) platinum (VI) chloride (MMP chloride) comes out by total energy which equalto-1209.074 a.u.

ACKNOWLEDGEMENTS

I am highly obligated to Prof. Dr. Abbas Abed Ali Drea for extending to me his all-out academic support throughout the course of this research. His keen interest in this work fructified as valuable guidance and positive criticism without which many constructive changes could not have directed this study also teaching me a new field of knowledge. My research ability has been enhanced by his in-depth knowledge. Also, I have learned and practiced conducting research in a systematic way under his supervision. My written communication skills have been improved significantly through his assistance.

I wish to thank university of Babylon, the college of science and the department of chemistry for giving me a chance to get this degree. I would like to extend my sincere appreciation to my mother and sister for their sacrifice, encouragement and inspiration. Without their generosity, it was not possible for me to conduct and complete this endeavor. Also, my great thanks Dr. Bahjat Razak Jaafar, Bahjat Mohammed Ali Said and Yahya Fahim for helping me. Finally, i would like to thank my family who have encouraged me throughout the past 3 years.

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