

# Molecular structure, vibrational spectra and electronic properties of cis-[Pt(2-aminothiazole)<sub>2</sub>Cl<sub>2</sub>]

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**Abstract**—Cis-[Pt(2-aminothiazole)<sub>2</sub>Cl<sub>2</sub>] was obtained. The geometry optimization of this molecule was done by Density Functional Theory (DFT/B3LYP) method with 6-31G(d) basis set and LANL2DZ for Pt. The experimental infrared spectrum was compared with calculated and complete vibrational assignment was provided. The bond orders and the electronic properties of the molecule were calculated. The natural bond orbital analysis (NBO) was performed in order to study the intramolecular bonding interactions among bonds and delocalization of unpaired electrons. The calculated highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) with frontier orbital gap were presented.

**Keywords**—cis-[Pt(2-aminothiazole)<sub>2</sub>Cl<sub>2</sub>], quantum chemical calculations, geometry optimization, electronic properties

## I. INTRODUCTION

The thiazoles compounds have a number of characteristic pharmacological features, such as relative stability and ease of starting materials. 2-Aminothiazoles are known mainly as biologically active compounds with a broad range of activity and as intermediates in the synthesis of antibiotics and dyes [1]. The biological activity of these compounds may be connected to their ability [2, 3] to form complexes with metal ions. Metal complexes with these ligands are becoming important as biochemical and antimicrobial reagents [4, 5]. Cis-platin has a significant activity against a variety of tumors. There is a continuing interest in the development of new platinum complexes, which are less toxic and noncross-resistance to cisplatin. Large part of the platinum complexes exhibiting antitumor activity have two cis ligands, such as chlorides and two strongly bonded amine type groups [6, 7].

The aims of the present work are using quantum chemical calculations to determine the geometry and electronic structure of cis-[Pt(2-aminothiazole)<sub>2</sub>Cl<sub>2</sub>], to provide vibrational assignment for the IR spectra and investigate quantum chemical parameters, such as highest occupied, lowest unoccupied molecular orbital energy levels, energy gap, atomic charges.

## II. EXPERIMENTAL

The cis-[Pt(2-aminothiazole)<sub>2</sub>Cl<sub>2</sub>] was obtained by mixing water solutions of (NH<sub>4</sub>)<sub>2</sub>PtCl<sub>4</sub> and of 2-Aminothiazole in mol ratio 1:2. The crystalline product which precipitated slowly (after one week) was filtered off and washed with water and dried under vacuum. The infrared spectra were recorded on a Bruker Tensor 27 FT-IR spectrometer in the 4000 – 400 cm<sup>-1</sup> range, with the samples embedded in KBr matrixes.

## III. COMPUTATIONAL METHODS

The full optimization of cis-[Pt(2-aminothiazole)<sub>2</sub>Cl<sub>2</sub>] was carried out by Density Functional Theories (DFT) method using Gaussian 03 software [8]. It was used Becke's three parameter hybrid exchange functional with Lee–Yang–Parr correlation functional (B3LYP) [9-11] with added polarization functions for H, S, C, N и Cl – 6-31G(d) and LANL2DZ [12-14] for Pt. All calculations were converged to 10<sup>-8</sup> a.u. Vibrational analysis was performed at each stationary point found, that confirm its identity as an energy minimum.

The population analysis was performed by the natural bond orbital method [15] at B3LYP/6-31G(d) level of theory using NBO program [16] under Gaussian 2003 program package. Natural bond orbital analysis stresses the role of intermolecular orbital interaction in the complex, particularly charge transfer. This is carried out by considering all possible interactions between filled donor and empty acceptor orbitals and estimating their energetic importance by second-order perturbation theory. For each filled orbital of the donor ( $\Phi_i$ ) and the empty orbital of the acceptor ( $\Phi_j$ ), the stabilization energy ( $\Delta E_{ij}^{(2)}$ ) associated with electron delocalization between donor and acceptor and it is calculated by equation (1) [17].

$$\Delta E_{ij}^{(2)} = q_i \frac{\langle \phi_i | F_{ij} | \phi_j \rangle^2}{\varepsilon_j - \varepsilon_i}, \quad (1)$$

where  $q_i$  is the donor orbital occupancy,  $\varepsilon_i$  and  $\varepsilon_j$  are NBO energies,  $F_{ij}$  is Fock matrix element between the  $i$  and  $j$  NBO orbitals. NBO analysis reveals the intra- and intermolecular interactions, it is one of the appropriate methods for investigating hyper conjugative interactions.

## IV. RESULTS AND DISCUSSION

## A. Geometry Optimization

The equilibrium geometry was determined by the energy minimization. The ground state optimized geometrical structure and atomic labeling of cis-[Pt(2-aminothiazole)<sub>2</sub>Cl<sub>2</sub>] are shown in Figure 1.

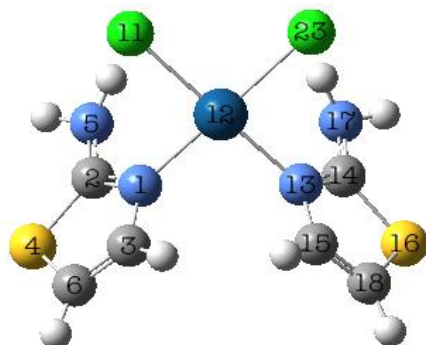


Figure 1. Optimized geometrical structure and atomic labeling of cis-[Pt(2-aminothiazole)<sub>2</sub>Cl<sub>2</sub>]

(C-atoms are in grey, Cl-atoms are in green, S-atoms are in yellow, N-atoms are in blue, Pt-atom is in dark blue, H-atoms are in white)

Table 1. Some optimized geometrical parameters of cis-[Pt(2-aminothiazole)<sub>2</sub>Cl<sub>2</sub>]

Parameters			
Bond length (Å)		Bond angle (degree)	
Pt-Cl <sup>11(23)</sup>	2.363	N <sup>1</sup> -Pt-N <sup>13</sup>	92.3
Pt-N <sup>1(13)</sup>	2.084	C <sup>2(14)</sup> -S <sup>4(16)</sup> -C <sup>6(18)</sup>	89.6
S <sup>4(16)</sup> -C <sup>2(14)</sup>	1.752	Pt-N <sup>1(13)</sup> -C <sup>2(14)</sup>	122.9
S <sup>4(16)</sup> -C <sup>6(18)</sup>	1.750	Pt-N <sup>1(13)</sup> -C <sup>3(15)</sup>	125.1
C <sup>2(14)</sup> -N <sup>5(17)</sup>	1.357	C <sup>2(14)</sup> -N <sup>1(13)</sup> -C <sup>3(15)</sup>	112.0
N <sup>1(13)</sup> -C <sup>2(14)</sup>	1.326	S <sup>4(16)</sup> -C <sup>2(14)</sup> -N <sup>5(17)</sup>	122.7
N <sup>1(13)</sup> -C <sup>3(15)</sup>	1.388	S <sup>4(16)</sup> -C <sup>2(14)</sup> -N <sup>1(13)</sup>	112.9
C <sup>3(15)</sup> -C <sup>6(18)</sup>	1.352	N <sup>5(17)</sup> -C <sup>2(14)</sup> -N <sup>1(13)</sup>	124.3
<b>Bond angle (degree)</b>		N <sup>1(13)</sup> -C <sup>3(15)</sup> -C <sup>6(18)</sup>	115.6
Cl <sup>11</sup> -Pt-Cl <sup>23</sup>	91.8	S <sup>4(16)</sup> -C <sup>6(18)</sup> -C <sup>3(15)</sup>	109.9
N <sup>1(13)</sup> -Pt-Cl <sup>11(23)</sup>	87.9	C <sup>3(15)</sup> -N <sup>1(13)</sup> -Pt-Cl <sup>23(11)</sup>	162.2
N <sup>1(13)</sup> -Pt-Cl <sup>23(11)</sup>	178.0	N <sup>5(17)</sup> -C <sup>2(14)</sup> -N <sup>1(13)</sup> -Pt	0.3

Table 2. Mulliken atomic charges and bond orders of cis-[Pt(2-aminothiazole)<sub>2</sub>Cl<sub>2</sub>]

Atom	Mulliken atomic charges	Bond	Bond order
Pt	0.027	Pt-Cl <sup>11(23)</sup>	1.249
Cl <sup>11(23)</sup>	-0.249	Pt-N <sup>1(13)</sup>	0.746
N <sup>1(13)</sup>	-0.493	S <sup>4(16)</sup> -C <sup>2(14)</sup>	1.252
N <sup>5(17)</sup>	-0.724	S <sup>4(16)</sup> -C <sup>6(18)</sup>	1.230
S <sup>4(16)</sup>	0.269	C <sup>2(14)</sup> -N <sup>5(17)</sup>	1.416
C <sup>2(14)</sup>	0.311	N <sup>1(13)</sup> -C <sup>2(14)</sup>	1.530
C <sup>3(15)</sup>	0.110	N <sup>1(13)</sup> -C <sup>3(15)</sup>	1.259
C <sup>6(18)</sup>	-0.369	C <sup>3(15)</sup> -C <sup>6(18)</sup>	1.782

The results obtained from the geometry optimization of cis-[Pt(2-aminothiazole)<sub>2</sub>Cl<sub>2</sub>] in gas-phase cannot be verified experimentally. The optimized structural parameters (bond lengths, bond

angles, dihedral angles) of cis-[Pt(2-aminothiazole)<sub>2</sub>Cl<sub>2</sub>] are listed in Table 1.

Quantum chemical calculations provide the ability to calculate the net atomic charges (*q*), which are localized at the corresponding atoms as a result of the redistribution of the electrons in the molecule. They allow the understanding of the distribution of the electronic density in a system of connected atoms and predict some chemical properties of the molecules. The atomic charge values were obtained by the Mulliken population analysis [18]. The net atomic charges and the order of the bonds in the investigated compound are presented in Table 2.

## B. Natural Bond Orbital Analysis

NBO analysis is an efficient method for study of the intra-molecular and inter-molecular bonding and interactions among bonds, and also provides a convenient basis for investigation charge transfer or conjugative interactions in molecular systems.

Calculations were performed using the Gaussian 03 package at the DFT/B3LYP/6-31G(d) level of the theory with LANL2DZ for Pt. Table 3 lists the calculated occupancies of natural orbitals. The calculated natural hybrids on atoms are also given in this table. As seen from Table 3, the σ(N<sup>1(13)</sup>-Pt) bond is resulting from the overlap of an sp<sup>2.45</sup> hybrid on nitrogen with an sp<sup>2.04</sup>d<sup>1.24</sup> hybrid on platinum. The higher electronegativity of the nitrogen atom is reflected in the larger percentage (85.46) for the nitrogen hybrid. On the other hand, σ(Cl<sup>11(23)</sup>-Pt) bond is formed from an sp<sup>4.95</sup> hybrid on chlorine atom and sp<sup>2.23</sup>d<sup>1.11</sup> hybrid on platinum – 79.04% of the bond is contributed from the Cl orbital, while 20.96% of the bond comes from the platinum orbital.

In the NBO method, delocalization of electron density (ED) between occupied Lewis-type orbitals and formally unoccupied (antibonding or Rydberg) non-Lewis NBOs corresponds to a stabilizing donor-acceptor interaction. The strength of this interaction can be estimated by the second order perturbation theory. Thus, the results obtained from NBO analysis provide convenient basis for investigating conjugative interactions in molecular systems. The larger stabilization energy *E*<sup>(2)</sup> value, the more intensive is the interaction between electron donors and acceptors, i.e. the more electron donating tendency from electron donors to acceptors and the greater the extent of conjugation of the whole system. This interaction results a loss of occupancy from the concentration of electron NBO of the idealized Lewis (bond or lone pair) structure into an empty (anti-bond or Rydberg) non-Lewis orbital. The second-order perturbation theory analysis of Fock matrix in NBO basis of cis-[Pt(2-aminothiazole)<sub>2</sub>Cl<sub>2</sub>] display strong intra-molecular conjugative and hyperconjugative interactions and delocalization of electron density within the molecule.

In NBO analysis large *E*<sup>(2)</sup> value shows the intensive interaction between electron-donors and electron-acceptors, and greater the extent of conjugation of the whole system. Some important

interactions between Lewis and non-Lewis orbitals along with their interacting stabilization energies are shown in Table 4.

The second-order perturbation theory analysis of Fock-matrix in NBO basis shows that strong intramolecular conjugative interactions are formed by orbital overlap between  $n(N^{5(17)})$  and  $\pi^*(N^{1(13)}-C^{2(14)})$ , and that between  $n(S^{4(16)})$  and  $\pi^*(N^{1(13)}-C^{2(14)})$ , bond orbital which result in stabilization of the system. There occurs a strong intramolecular conjugative interaction of  $N^{1(13)}-C^{2(14)}$  from  $N^{5(17)}$  and from  $S^{4(16)}$  of  $n1(N^{5(17)}) \rightarrow \pi^*(N^{1(13)}-C^{2(14)})$  and of  $n2(S^{4(16)}) \rightarrow \pi^*(N^{1(13)}-C^{2(14)})$ ,

which increases ED(0.498e) leading to stabilization of 46.06 and 32.61 kcal/mol. Also there occurs a strong intramolecular hyper conjugative interaction of  $Pt-N^{1(13)}$  from  $Pt-Cl^{11(23)}$  of  $\sigma(Pt-Cl^{11(23)}) \rightarrow \sigma^*(Pt-N^{1(13)})$  which increases ED(0.153e) that weakens the respective bonds  $Pt-Cl^{11(23)}$  (1.880e) leading to stabilization of 20.13 kcal/mol and also the hyper conjugative interaction of  $\sigma(Pt-N^{1(13)}) \rightarrow \sigma^*(Pt-Cl^{11(23)})$  leading to stabilization of 19.60 kcal/mol. The conjugative interaction of  $\pi(N^{1(13)}-C^{2(14)}) \rightarrow \pi^*(C^{3(15)}-C^{6(18)})$ ;  $\pi(N^{1(13)}-C^{2(14)}) \rightarrow \pi^*(C^{3(15)}-C^{6(18)})$  leading to stabilization of 18.86 and 32.03 kcal/mol respectively.

Table 3. Occupancy of natural orbitals (NBOs) and hybrids of cis-[Pt(2-aminothiazole)<sub>2</sub>Cl<sub>2</sub>] by the B3LYP method with 6-31G(d) basis set and LanL2dz for Pt atom

Bond orbital	Occupancy	Hybrids <sup>a</sup>	AO (%) <sup>b</sup>
$\sigma N^{1(13)}-C^{2(14)}$	1.985	$sp^{1.79}(N^{1(13)}) + sp^{1.83}(C^{2(14)})$	60.63%(N <sup>1(13)</sup> ) + 39.37%(C <sup>2(14)</sup> )
$\pi N^{1(13)}-C^{2(14)}$	1.889	$p(N^{1(13)}) + p(C^{2(14)})$	66.67%(N <sup>1(13)</sup> ) + 33.33%(C <sup>2(14)</sup> )
$\sigma N^{1(13)}-C^{3(15)}$	1.980	$sp^{1.84}(N^{1(13)}) + sp^{2.59}(C^{3(15)})$	61.90%(N <sup>1(13)</sup> ) + 38.10%(C <sup>3(15)</sup> )
$\sigma N^{1(13)}-Pt$	1.878	$sp^{2.45}(N^{1(13)}) + sp^{2.04}d^{1.24}(Pt)$	85.46%(N <sup>1(13)</sup> ) + 14.54%(Pt)
$\sigma C^{2(14)}-S^{4(16)}$	1.975	$sp^{2.42}(C^{2(14)}) + sp^{4.88}(S^{4(16)})$	54.15%(C <sup>2(14)</sup> ) + 45.85%(S <sup>4(16)</sup> )
$\sigma C^{2(14)}-N^{5(17)}$	1.993	$sp^{1.83}(C^{2(14)}) + sp^{1.80}(N^{5(17)})$	41.04%(C <sup>2(14)</sup> ) + 58.96%(N <sup>5(17)</sup> )
$\sigma C^{3(15)}-C^{6(18)}$	1.985	$sp^{1.60}(C^{3(15)}) + sp^{1.53}(C^{6(18)})$	49.66%(C <sup>3(15)</sup> ) + 50.34%(C <sup>6(18)</sup> )
$\pi C^{3(15)}-C^{6(18)}$	1.933	$p(C^{3(15)}) + p(C^{6(18)})$	45.27%(C <sup>3(15)</sup> ) + 54.73%(C <sup>6(18)</sup> )
$\sigma S^{4(16)}-C^{6(18)}$	1.976	$sp^{4.54}(S^{4(16)}) + sp^{3.06}(C^{6(18)})$	48.69%(S <sup>4(16)</sup> ) + 51.31%(C <sup>6(18)</sup> )
$\sigma Cl^{11(23)}-Pt$	1.881	$sp^{4.95}(Cl^{11(23)}) + sp^{2.23}d^{1.11}(Pt)$	79.04%(Cl <sup>11(23)</sup> ) + 20.96%(Pt)

a Hybrids on atoms.

b Percentage contribution of atomic orbitals in NBO hybrid.

Table 4. Second-order perturbation theory analysis of Fock matrix in NBO basis

Donor NBO (i)	ED (i)/e	Acceptor NBO (j)	ED (j)/e	E <sup>(2)</sup> kcal/mol	E(j) – E(i) a.u.	F(i,j) a.u.
$\pi N^1-C^2$	1.889	$\pi^* C^3-C^6$	0.241	18.86	0.36	0.076
$\sigma N^1-Pt$	1.878	$\sigma^* Pt-Cl^{23}$	0.098	19.60	0.67	0.103
$\sigma Cl^{11}-Pt$	1.881	$\sigma^* Pt-N^{13}$	0.153	20.13	0.65	0.103
$\sigma Pt-N^{13}$	1.878	$\sigma^* Cl^{11}-Pt$	0.098	19.61	0.67	0.103
$\sigma Pt-Cl^{23}$	1.880	$\sigma^* N^1-Pt$	0.153	20.13	0.65	0.103
$\pi N^{13}-C^{14}$	1.889	$\pi^* C^{15}-C^{18}$	0.241	18.86	0.36	0.076
$n2 S^4$	1.678	$\pi^* N^1-C^2$	0.498	32.61	0.22	0.080
$n2 S^4$	1.678	$\pi^* C^3-C^6$	0.241	17.55	0.27	0.063
$n1 N^5$	1.762	$\pi^* N^1-C^2$	0.498	46.07	0.26	0.105
$n2 S^{16}$	1.678	$\pi^* N^{13}-C^{14}$	0.498	32.61	0.22	0.080
$n2 S^{16}$	1.678	$\pi^* C^{15}-C^{18}$	0.241	17.55	0.27	0.063
$n1 N^{17}$	1.762	$\pi^* N^{13}-C^{14}$	0.498	46.06	0.26	0.105
$\pi^* N^1-C^2$	0.498	$\pi^* C^3-C^6$	0.241	32.02	0.05	0.060
$\pi^* N^{13}-C^{14}$	0.498	$\pi^* C^{15}-C^{18}$	0.241	32.03	0.05	0.060

E<sup>(2)</sup> – means energy of hyper-conjugative interactions (stabilization energy) in kcal/mol.

E(j) – E(i) – Energy difference between donor and acceptor i and j NBO orbitals in a.u.

F(i, j) – is the Fock matrix elements between i and j NBO orbitals in a.u.

### C. Homo-Lumo Analysis

The frontier orbitals (highest occupied molecular orbital – HOMO and lowest unoccupied molecular orbital – LUMO) are very important in defining reactivity. The HOMO exhibits the ability to donate an electron and LUMO as an electron acceptor serves the ability to obtain an electron. The frontier orbitals (HOMO, LUMO) of cis-[Pt(2-aminothiazole)<sub>2</sub>Cl<sub>2</sub>] calculated by B3LYP/6-31G(d) and LANL2DZ for Hf are plotted in Figure 2.

Energy of frontier orbitals and energy of the gap are:

$$E_{\text{HOMO}} = -581.680 \text{ kJ/mol}$$

$$E_{\text{LUMO}} = -147.107 \text{ kJ/mol}$$

$$\Delta E_{\text{LUMO-HOMO}} = 434.573 \text{ kJ/mol}$$

High values of  $E_{\text{HOMO}}$  have a tendency of the molecule to donate electrons to appropriate acceptor molecules with low energy, empty molecular orbitals. The energy of the lowest unoccupied molecular orbital indicates the ability of the molecule to accept electrons. The lower value of  $E_{\text{LUMO}}$ , the more probable it is that the molecule would accept electrons. Consequently, concerning the value of the energy of the gap  $\Delta E_{\text{LUMO-HOMO}}$ , larger values of the energy difference will provide low reactivity to a chemical species. Lower values of the energy difference will render good

inhibition efficiency, because the energy to remove an electron from the last occupied orbital will be low. The results for the calculations of the ionization potential ( $I$ ) and the electron affinity ( $A$ ) by application of the Koopman's theorem [19] are shown. According to the Hartree–Fock theorem, the frontier orbital energies are given by:  $I = -E_{\text{HOMO}} = 581.680$  kJ/mol;  $A = -E_{\text{LUMO}} = 147.107$  kJ/mol. This theorem establishes a relation between the energies of the HOMO and the LUMO and the ionization potential and the electron affinity, respectively. Although no formal proof of this theorem exists within DFT, its validity is generally accepted. Electronegativity ( $\chi$ ), chemical potential ( $\mu$ ) and global hardness ( $\eta$ ), their operational and approximate definitions for cis-[Pt(2-aminothiazole)<sub>2</sub>Cl<sub>2</sub>] are:  $\chi = -\mu = (I + A)/2 = 364.394$  kJ/mol;  $\eta = (I - A)/2 = 217.287$  kJ/mol.

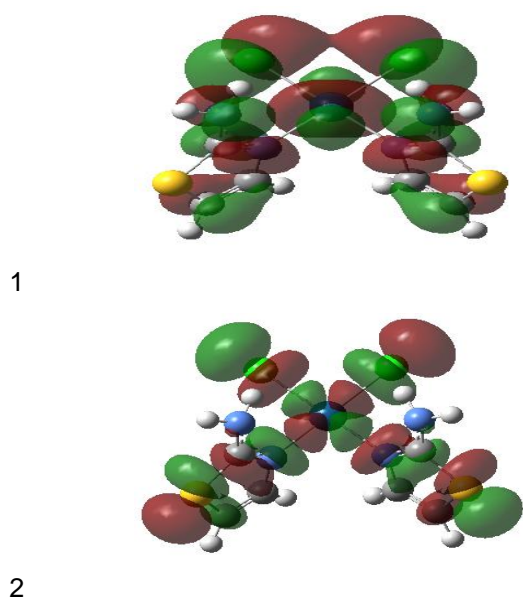


Figure 2. Electron distribution of HOMO – 1 and LUMO – 2 for cis-[Pt(2-aminothiazole)<sub>2</sub>Cl<sub>2</sub>]

#### D. Vibrational Spectral Analysis

The vibrational spectra of cis-[Pt(2-Aminothiazole)<sub>2</sub>Cl<sub>2</sub>] was calculated by DFT with B3LYP functional having extended basis sets 6-31G(d) and LANL2DZ for Pt. Frequencies recorded experimentally for cis-[Pt(2-Aminothiazole)<sub>2</sub>Cl<sub>2</sub>] are compared with the calculated obtained by DFT (Figure 3).

It is well known that the harmonic frequencies by DFT calculations are usually higher than the corresponding experimental quantities due to the facts

of the electron correlation approximate treatment, the anharmonicity effect and basis set deficiency, etc. [20]. In order to improve the calculated values in agreement with the experimental values, it is necessary to scale down the calculated harmonic frequencies. After scaling, the theoretical frequencies match well with the experimental ones. The experimental assignments of IR for vibrations, IR theoretical and relative intensities were reported in Table 5.

These assignments are important to understand the molecular structure of the title molecule. Any discrepancies noted between the observed and the calculated wavenumbers due to the fact that the calculations were actually performed on single (isolated) molecules in the gaseous state. Thus some reasonable deviations from the experimental values seem to be justified.

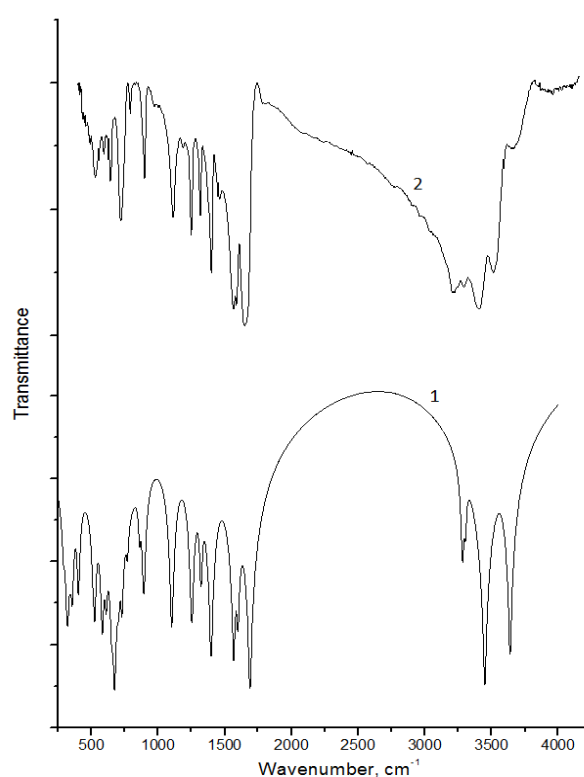


Figure 3. IR spectrum of cis-[Pt(2-Aminothiazole)<sub>2</sub>Cl<sub>2</sub>], 1 – calculated, 2 – experimental

Table 5. Experimental and calculated characteristic frequencies (cm<sup>-1</sup>), IR intensity and probable assignments of 2-Aminothiazole and cis-[Pt(2-Aminothiazole)<sub>2</sub>Cl<sub>2</sub>]

2-Aminothiazole			[Pt(2-Aminothiazole) <sub>2</sub> Cl <sub>2</sub> ]			Assignments <sup>b</sup>
Experimental frequencies[21] <sup>a</sup>	Calculated		Experimental frequencies	Calculated		
	Scaled	IAbs		Scaled	IAbs	
–	3686	29	3808 s	3638	72	$\nu_{\text{asym}}(\text{NH}); (\text{NH}_2)$
3413 w	3569	37	3385 s	3449	273	$\nu_{\text{sym}}(\text{NH}); (\text{NH}_2)$
3293 w	3224	10	3283; 3100	3283	8	$\nu(\text{C-H})$
1764 s	1653	186	–	1689	278	$\delta_{\text{b}}(\text{NH}_2); \nu(\text{C=N})$
1629 m	1588	73	1594	1597	35	$\delta_{\text{b}}(\text{NH}_2); \nu(\text{C=N}); \nu(\text{C=C})$
1527 m	1544	52	1510	1567	146	$\delta_{\text{b}}(\text{NH}_2); \nu(\text{C-N}); \nu(\text{C=C})$

1361 s	1359	44	–	1399	93	<i>Rband</i> ; $\nu_{(C-H)}$
1327 s	1305	54	1355	1394	57	<i>Rband</i> ; $\nu_{(C-H)}$
1277 ms	1243	24	1273	1255	47	$\delta_{t(NH2)}$ ; $\nu_{(C-N)}$ ; $\nu_{(C-H)}$
1070 s	1054	47	1206	1247	14	$\delta_{t(NH2)}$ ; <i>Rband</i>
–	–	–	1072	1100	40	$\delta_{t(NH2)}$ ; <i>Rband</i>
–	–	–	876	862	4	$\nu_{(C-H)}$
769 s	754	12	770	768	4	<i>Rband</i> ; $\nu_{(C-S)}$
709 s	700	13	–	729	37	<i>Rband</i> ; $\delta_{r(NH2)}$
695 ms	650	46	699	705	22	<i>Rband</i> ; $\nu_{(C-S)}$
661 vs	644	158	623	674; 653	352	<i>Rband</i> ; $\delta_{w(NH2)}$
542 s	556	61	583	583	68	<i>Rband</i> ; $\delta_{w(NH2)}$
517 ms	510	103	527	525	48	<i>Rband</i>
–	292	36	400[18] <sup>c</sup>	404	15	$\delta_{r(NH2)}$
–	–	–	–	356; 342	28	$\delta_{t(NH2)}$
–	–	–	300[22] <sup>c</sup>	324	42	$\nu_{sym}(Pt-Cl)$
–	–	–	290[22] <sup>c</sup>	317	28	$\nu_{assym}(Pt-Cl)$
–	–	–	225[22] <sup>c</sup>	293	6	$\nu_{(Pt-N)}$
–	–	–	185[22] <sup>c</sup>	187	5	$\nu_{(Pt-N)}$
–	–	–	168[22] <sup>c</sup>	170	2	$\nu_{(Pt-N)}$

Scale factors of 0.9613 for calculated frequencies with B3LYP/6-31G(d,p)

(a) s - strong; m - medium; w - weak; vw - very weak

(b)  $\nu$  - stretching; ss - symmetric; ass - asymmetric;  $\delta_b$  - bending;  $\delta_r$  - rocking;  $\delta_w$  - wagging;  $\delta_t$  - twisting; *Rband* - ring deformation

(c) These experimental frequencies are of  $[Zn(2-Aminothiazole)_2Cl_2] - \delta_{r(NH2)}$ ;  $\nu_{sym}(Zn-Cl)$ ;  $\nu_{assym}(Zn-Cl)$ ;  $\nu_{(Zn-N)}$  respectively

$I_{Abs}$  - Theoretical infrared intensities

## V. CONCLUSION

The geometry of *cis*-[Pt(2-Aminothiazole)<sub>2</sub>Cl<sub>2</sub>] was optimized with DFT/B3LYP methods using 6-31G(d) basis set and LANL2DZ for Pt. The complete molecular structural parameters of the compound were obtained. The vibrational frequencies of the fundamental modes of the compound were precisely assigned, analyzed and the theoretical results were compared with the experimental vibrations. The close agreement was observed between the experimental and scaled frequencies obtained using the basis set 6-31G(d). HOMO–LUMO studies reveal the intramolecular charge transfer through conjugated system. The Mulliken charges calculated by B3LYP/6-31G(d) method were presented. The transactions give stabilization to the structure were identified by second order perturbation energy calculations. Using NBO analysis the stability of the molecule arising from hyper-conjugative interaction and charge delocalization was analyzed. The present quantum chemical study may lead to the understanding of properties and activity of *cis*-[Pt(2-Aminothiazole)<sub>2</sub>Cl<sub>2</sub>].

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