A New Pt(II) Complex with Anionic s-Triazine Based NNO-Donor Ligand: Synthesis, X-ray Structure, Hirshfeld Analysis and DFT Studies

Mezna Saleh Altowyan, Saied M. Soliman, Jamal Lasri, Naser E. Eltayeb, Matti Haukka, and Ayman El-Faham

1. Introduction

s-triazine and their metal complexes have gained much attention for their properties and potential applications in many fields [1]. In the last decade, s-triazine and their complexes have been explored in the pharmaceutical field, catalytic process including Heck and Suzuki-Miyaura cross-coupling reactions, olefin polymerization, hydrogen transfer reactions, decarbonylation of ketones, asymmetric allylic alkylation, and some derivatives have been designed to develop photoelectronic materials [1]. Several ligands have been synthesized based on the s-triazine as a core structure and have been explored in coordination chemistry [1]. Mukherjee et al. constructed a complicated coordinated molecule by coordination-driven self-assembly of homometallic Pd/Pt-based s-triazine ligand as interlocked molecular cages [2]. Motloch et al. reported the synthesis of the Pt(II)/Pd(II) complex with s-triazine-type ligands for the purpose of hydrogen bonded/metal-coordination hybrid [3]. Another representative example was designed, synthesized and characterized by He et al. via self-assembly of supramolecular coordination complexes using platinum salt with two different types of pyridyl-derivatized ligands [4]. The photophysical properties of these supramolecular coordination complexes showed potential metal ion-responsive
properties of these supramolecular coordination complexes showed potential metal ion-coordination characteristics of the functional groups, e.g., NH (3428 cm\(^{-1}\)), aromatic C–H (3120 cm\(^{-1}\)), aliphatic C–H (2957 and 2866 cm\(^{-1}\)), C=N/C=C (1630 cm\(^{-1}\)).

2. Results and Discussion

2.1. [Pt(Triaz)Cl] Complex Synthesis and Characterization

The Pt(II) complex [Pt(Triaz)Cl] was synthesized by reaction of (HTriaz) ligand with platinum (II) chloride (1:1) in acetone under heating (Scheme 1). The new Pt(II) complex was characterized by FT-IR, UV-Vis, single-crystal X-ray diffraction and CHN/Pt analyses. The reported structure by single-crystal X-ray diffraction agreed very well with the elemental analysis results. Additionally, the FT-IR spectra of [Pt(Triaz)Cl] exhibited vibrational characteristics of the functional groups, e.g., NH (3428 cm\(^{-1}\)), aromatic C–H (3120 cm\(^{-1}\)), aliphatic C–H (2957 and 2866 cm\(^{-1}\)), C=N/C=C (1630 cm\(^{-1}\)).

During our study, we have explored the utility of the hydrazono-s-triazine-based ligand towards metalation with the divalent platinum ion to synthesize a new Pt(II) complex based on s-triazine hydrazone ligand (Figure 1). Its 3D molecular and supramolecular structures were elucidated by single-crystal X-ray diffraction and Hirshfeld analyses. The chemical insights of the Pt(II) complex have also been demonstrated.
2.2. Crystal Structure Description

The X-ray structure of \([\text{Pt(Triaz)}\text{Cl}]\) including atom numbering and thermal ellipsoids drawn at 50% probability level is shown in Figure 2 (upper part). The \([\text{Pt(Triaz)}\text{Cl}]\) complex crystallized in \(I \overline{2} a\) space group (Table S1; Supplementary data). The asymmetric unit comprised one \([\text{Pt(Triaz)}\text{Cl}]\) complex unit and one acetone as a crystal solvent. The ligand (\(\text{Triaz}^{-1}\)) is a \(NNO\) tridentate ligand. The donor atoms of this ligand are two nitrogen atoms from the \(s\)-triazine and the hydrazone fragments in addition to the phenolic oxygen atom. The coordination environment of the Pt(II) is completed by one Cl\(^{-1}\) trans to the Pt-N (hydrazone). The Pt to donor atoms (N4, N7, O2 and Cl1) distances are 2.055(4), 1.945(4), 1.991(4) and 2.331(1) Å, respectively. The angle between the trans-bonds O2-Pt1-N4 and N7-Pt1-Cl1 are 173.35(16) and 177.01(13) Å, respectively (Table 1). The results are in good agreement with the X-ray structure of the structurally related \([\text{Pd(Triaz)}\text{Cl}]\) complex [20].

Table 1. \([\text{Pt(Triaz)}\text{Cl}]\) complex bond lengths [Å] and angles [°].

| Atoms     | Distance | Atoms     | Distance |
|-----------|----------|-----------|----------|
| Pt1-N7    | 1.945(4) | Pt1-N4    | 2.055(4) |
| Pt1-O2    | 1.991(4) | Pt1-Cl1   | 2.3308(13) |
| Atoms     | Angle    | Atoms     | Angle    |
| N7-Pt1-O2 | 93.09(16)| N7-Pt1-Cl1| 177.01(13)|
| N7-Pt1-N4 | 80.42(18)| O2-Pt1-Cl1| 83.91(11) |
| O2-Pt1-N4 | 173.35(16)| N4-Pt1-Cl1| 102.58(13)|

On the other hand, the angles between the cis-bonds are in the range of 83.91(11)–102.58(13)°, indicating a distorted square planar coordination environment around the Pt(II). The structure of this complex showed one intramolecular N-H–O H-bond between the N–H group from the organic ligand as a H-bond donor and the carbonyl oxygen atom from the acetone molecule as H-bond acceptor. The hydrogen-acceptor and donor-acceptor distances are 2.028 and 2.777(7) Å, respectively, while the N6-H6–O3 angle is 141.6°. A view of packing along \(ac\)-plane is shown in the lower part of Figure 2.
Scheme 1. Synthesis of [Pt(Triaz)Cl] complex.

2.2. Crystal Structure Description

The X-ray structure of [Pt(Triaz)Cl] including atom numbering and thermal ellipsoids drawn at 50% probability level is shown in Figure 2 (upper part). The [Pt(Triaz)Cl] complex crystallized in I2/a space group (Table S1; Supplementary data). The asymmetric unit comprised one [Pt(Triaz)Cl] complex unit and one acetone as a crystal solvent. The ligand (Triaz$^-1$) is a NNO tridentate ligand. The donor atoms of this ligand are two nitrogen atoms from the $s$-triazine and the hydrazone fragments in addition to the phenolic oxygen atom. The coordination environment of the Pt(II) is completed by one Cl$^-1$ trans to the Pt-N (hydrazone). The Pt to donor atoms (N4, N7, O2 and Cl1) distances are 2.055(4), 1.945(4), 1.991(4) and 2.331(1) Å, respectively. The angles between the trans-bonds O2-Pt1-N4 and N7-Pt1-Cl1 are 173.35(16) and 177.01(13) Å, respectively (Table 1). The results are in good agreement with the X-ray structure of the structurally related [Pd(Triaz)Cl] complex [20].

Figure 2. X-ray structure (upper) and packing view along ac-plane (lower) for [Pt(Triaz)Cl] complex.

2.3. Analysis of Molecular Packing

Hirshfeld surfaces mapped over $d_{\text{norm}}$, shape index (SI) and curvedness for the studied complex are shown in Figure 3, while the different contacts and their contribution percentages in the molecular packing are present in Figure 4.

As can be seen from Figure 4, the most dominant interactions are the H···H, H···C and O···H intermolecular contacts. These interactions contributed 60.9, 11.2, and 8.3% of the whole fingerprint area while the corresponding values for the Pd(II) complex are 60.6, 11.6, and 8.1, respectively. Other minor contributions from the Cl···H, C···N, N···H and C···C contacts were also detected. Generally, the most significant contacts are the O···H and H···C interactions. The latter belongs to the C-H···π interactions. In the corresponding Pd(II) complex, the O···H, H···H and H···C interactions are the most important. These intermolecular contacts appeared as red spots in $d_{\text{norm}}$ and characterized by spikes in the fingerprint plots as shown in Figure 5. The O···H interactions appeared as one spike in the upper left part of the fingerprint plot due to the N–H···O (1.934 Å) and C–H···O (2.416 Å) interactions between the carbonyl group as hydrogen bond acceptor and the surface as hydrogen bond donor. On the other hand, the C–H···π interactions are characterized by two
spikes with interaction distances ranges from 2.630 Å (H4A···C15) to 2.785 Å (H19B···C16). In the corresponding Pd(II) complex, the O···H and H···C interactions are 1.839 and 2.608 Å, respectively which are slightly shorter than the corresponding values of the [Pt(Triaz)Cl] complex. In the former, all H···H interactions have long interaction distances while in the latter, most H···H interactions also have long interaction distances, except for the H11···H2B contact, which appeared as a red spot in the $d_{\text{norm}}$. The H11···H2B contact distance is 2.003 Å. A summary of all contacts with shorter distances than the vdW radii sum of the interacting elements is listed in Table 2.

**Figure 3.** Hirshfeld surfaces of [Pt(Triaz)Cl].

![Hirshfeld surfaces of [Pt(Triaz)Cl]](image-url)
well with the experimental X-ray structure (Table S2, Supplementary data). In addition, the extra stability of the complexation of the ligand with Pt(II) decreased the polarity of the system. The calculated dipole moments are 7.933 and 2.289 Debye, respectively. It is clear that the ligand and its Pt(II) complex are polar compounds where the calculated dipole moments are 7.933 and 2.289 Debye, respectively. It is clear that the ligand and its Pt(II) complex are polar compounds where the calculated dipole moments are 7.933 and 2.289 Debye, respectively.
Figure 5. $d_{\text{norm}}$ maps (right) and fingerprint plots (left) of the O···H, H···C and H···H contacts in [Pt(Triaz)Cl].

2.4. DFT Studies

The optimized structures of [Pt(Triaz)Cl] and two possible geometrical isomers (F1 (E) and F2 (Z); Figure 1) of the free ligand are shown in Figure 6. The total energies of the ligand isomers are $-1622.4327$ and $-1622.4126$ a.u. for F1 and F2, respectively. Hence, F1 is the more stable than F2 by 12.6019 kcal/mol. This result agreed with our previous
The calculated charge at Pt, Cl and the anionic ligand. Table 3.

The interaction between Pt(II) as a Lewis acid and ligand as a Lewis base affect the net charge at both fragments. The calculated charges at Pt, Cl, and the anionic ligand are depicted in Table 3. The charge at the Pt(II) is changed to +0.5 instead of +2.0 due to the large electron density transferred from the ligand groups. The amount of negative electron density transferred from the ligand groups are 0.56 and 0.95 e for the Cl$^-1$ and Triaz$^-1$, respectively.

Table 3. The calculated charge at Pt, Cl and the anionic ligand.

| Atom/Group | Optimized | X-ray |
|------------|-----------|-------|
| Pt         | 0.4998    | 0.4857|
| Cl         | −0.4410   | −0.4402|
| Triaz      | −0.0588   | −0.0455|

2.5. UV–Vis Spectra

The experimental and calculated UV–Vis spectra of the studied Pt(II) complex in ethanol as solvent are presented in Figure 8. The longest wavelength band was observed experimentally at 427 nm. The TD-DFT calculations predicted this band at 409 nm with
oscillator strength of 0.1646. This electronic transition was assigned to HOMO→LUMO (93%) excitation. In addition, the TD-DFT calculations predicted intense absorptions at 322 nm (exp. 338 nm) and 305 nm (exp. 320 nm) with oscillator strengths of 0.2102 and 0.2196, respectively. These electronic transition bands were assigned to H−1→LUMO (83%) and HOMO→L+2 (84%), respectively. Experimentally, the region below 300 nm showed an intense absorption at 261 nm, which is calculated at 266 nm (f = 0.3628). This band was assigned to H−1→L+2 (89%) excitation. Presentation of molecular orbitals (MOs) included in these electronic transitions are shown in Figure 9. Theoretically, an absorption band and a shoulder were predicted at 247 nm (f = 0.1883) and 226 nm (f = 0.1040), respectively. The former was assigned to the mixed H−3→L+2 (56%) and HOMO→L+5 (11%) transitions while the latter was assigned for H−3→L+3 (26%) and HOMO→L+6 (17%)/L+7 (35%) transitions.

Figure 8. The experimental (left) and calculated (right) UV–Vis spectra of the studied [Pt(Triaz)Cl] complex.

Figure 9. The MOs included in the electronic transitions of the studied [Pt(Triaz)Cl] complex.
3. Materials and Methods

3.1. Materials and Methods

Chemicals were purchased from Sigma–Aldrich (Chemie GmbH, 82024 Taufkirchen, Germany). The CHN analyses were determined using Perkin–Elmer 2400 instrument (PerkinElmer, Inc. 940 Winter Street, Waltham, MA, USA). Pt content was determined using a Shimadzu atomic absorption spectrophotometer (AA-7000 series, Shimadzu, Ltd., Japan). FT-IR spectrum was assessed on a Perkin–Elmer 1000 FT-IR spectrometer, Waltham, MA, USA (Figure S1). The UV–Vis electronic spectrum of the Pt(II) complex at $3.0 \times 10^{-4}$ mol L$^{-1}$ in absolute ethanol as solvent was carried out using a UV–Vis spectrophotometer (Perkin–Elmer Lambda 35, Waltham, MA, USA) in 1 cm cell in the spectral range of 200–500 nm. Mass spectrum was recorded on JMS-600 H JEOL spectrometer (JEOL Ltd., Tokyo, Japan). $^1$H and $^{13}$C NMR spectra of [Pt(Triaz)Cl] were recorded on DMSO-$d_6$ using a JEOL 500 MHz spectrometer (JEOL Ltd., Tokyo, Japan) at room temperature.

3.2. Synthesis of the Ligand (HTriaz)

The ligand (HTriaz) has been prepared using our published method [20, 22] and the NMR spectral data agreed with the reported data [20].

3.3. Synthesis of [Pt(Triaz)Cl] Complex

The (HTriaz) ligand (60.0 mg, 0.119 mmol) was dissolved in 30 mL of acetone then PtCl$_2$ (31.6 mg, 0.119 mmol) was added. The reaction mixture was heated at 50 °C for 4 days. Then, the resulting solution mixture was filtered, and the filtrate was left for slow evaporation at room temperature to afford the final product [Pt(Triaz)Cl] as reddish-brown block crystals. Yield; C$_{31}$H$_{42}$ClN$_7$O$_3$Pt 79%; Anal. Calcd. for: C, 47.06; H, 5.35; N, 12.39; Pt, 24.65. Found: C, 47.24; H, 5.29; N, 12.20; Pt, 24.46. FT-IR (KBr) cm$^{-1}$: 3428 (NH), 3263, 3120, 2957, 2866 (C–H), 1540 and 1630 (C=N and C=C) (Figure S1; Supplementary data); $^1$H NMR (500 MHz, DMSO-$d_6$, ppm): $\delta$ 1.24 (s, 9H, 3CH$_3$), 1.37 (s, 9H, 3CH$_3$), 3.64 (t, 4H, $J = 4.0$ Hz, 2CH$_2$ (morpholine ring), 3.71 (t, 4H, $J = 3.6$ Hz, 2CH$_2$ (morpholine ring), 7.14 (t, 1H, $J = 6.8$ Hz, C$_6$H$_5$), 7.30 (d, 1H, $J = 2.0$ Hz, C$_6$H$_5$), 7.30–7.35 (m, 3H, C$_6$H$_5$ and C$_6$H$_2$), 7.63–7.57 (m, 3H, C$_6$H$_5$ and C$_6$H$_2$ and CH=N), 8.46 (s, 1H, NH), 10.91 (s, 1H, NH) (Figure S2; Supplementary data); $^{13}$C NMR (126 MHz, DMSO-$d_6$) $\delta$ 194.92, 178.15, 166.74, 164.72, 143.14, 141.50, 140.00, 138.81, 133.36, 131.26, 130.51, 128.42, 125.73, 125.09, 124.80, 123.88, 123.08, 122.93, 116.34, 116.17, 111.63, 74.32, 74.26, 62.38, 54.28, 49.14, 47.13, 36.54 (Figure S3; Supplementary data).

3.4. X-ray Structure Determinations

The details of the crystal structure determination are found in Table S1 and all technical experiments are provided in the supplementary materials [23–27].

3.5. Hirshfeld and DFT Calculations

Crystal Explorer 17.5 [28] was used to perform the analysis of molecular packing. Details of DFT and TD-DFT calculations [29–34] as well as proton affinity [35] are given in supplementary data.

4. Conclusions

A novel Pt(II) complex [Pt(Triaz)Cl] with tridentate NNO-donor ligand-based s-triazine scaffold was achieved. The chemical structure of [Pt(Triaz)Cl] was confirmed by CHNPt analyses and single-crystal X-ray diffraction. The Pt(II) coordination environment is distorted square planar. The structure of this complex showed one intramolecular N–H···O hydrogen bond between the N–H group from the organic ligand as a hydrogen bond donor and the carbonyl oxygen atom from the acetone molecule as a hydrogen bond acceptor. The supramolecular structure of the studied Pt(II) complex is analyzed using Hirshfeld calculations. Additionally, the calculated UV–Vis spectra were assigned based on the results of the TD-DFT calculations. The natural charges were calculated, and the results
indicated that the amount of the electron transfer from the Cl⁻⁻ and Triaz⁻⁻ is 0.56 and 0.95 e, respectively.

**Supplementary Materials:** The following supporting information can be downloaded online. Table S1: Crystal data and structure refinement for [Pt(Triaz)Cl]; Table S2. The calculated geometric parameters of [Pt(Triaz)Cl]; Figure S1: FT-IR spectra of the studied Pt(II) complex; Figure S2: ¹H NMR spectra of the studied Pt(II) complex; Figure S3: ¹³C NMR spectra of the studied Pt(II) complex.

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**Sample Availability:** Samples of the compound [Pt(Triaz)Cl] is available from the authors.

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