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ORIGINAL ARTICLE

# PCM, ETS-NOCV, and CDA investigations of interactions of a Cycloplatinated Thiosemicarbazone as antiparasitic and antitumor agents with $C_{20}$ nano-cage

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**Abstract**
In this work, we reported a computational investigation on the interaction between a cycloplatinated thiosemicarbazone (CT) as antiparasitic and antitumor agents with $C_{20}$ molecule. The solvent impacts were considered by the SCRF based on PCM. The relationships of solvation energies, interaction energy, dipole moment, and N-H stretching frequencies (ν(NH)) values with *modified-Buckingham* function were illustrated. ETS-NOCV, CDA, and EDA results provided valuable understanding into the interaction between two fragments.

**Keywords:** *Cycloplatinated Thiosemicarbazones; C20 Molecule; Charge Decomposition Analysis (CDA); Energy Decomposition Analysis (EDA); Extended Transition State-Natural Orbitals for Chemical Valence (ETS-NOCV); Polarizable Continuum Model (PCM).*

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## INTRODUCTION

Thiosemicarbazones ligands formed various complexes with metals. These molecules have been considered as antiparasitics [1, 2], antitumoral [3-7], antibacterial [8, 9] agents.

Nano-cages have been considered as significance drug delivery systems [10]. The $C_{20}$ molecule is the smallest fullerene [11] and computational investigations have been provided deep insights its properties [12-22]. A DFT study of the solvent effect, features, structures, together with topologies of the interaction between the $C_{20}$ Cage and cisplatin has been reported [23].

Significant effects of solvents in various fields of chemistry have been revealed [24-26]. Quantum mechanical researches are helpful to inspect the solvent consequence in the structural and properties of numerous molecules [27, 28]. Many computational reports have been employed to illustration of solvent effects on the structural and properties of inorganic and organometallic complexes [29-42].

Cycloplatinated thiosemicarbazone complexes from 3, 4-dichloroacetophenone thiosemicarbazone have been prepared [43]. Two complexes of them are indicated in Fig. 1. Computational illustration of Interaction of a cycloplatinated thiosemicarbazone as antitumor and antiparasitic agents with $B_{12}N_{12}$ nano-Cage has been reported [44].

In this work, the interaction of similar complex (CT) of this category and $C_{20}$ molecule has been reported (Fig. 2), and the solvent influence on the structure and properties of the complex was exemplified. CT...$C_{20}$ interaction was illustrated with using energy decomposition analysis (EDA) and extended transition state-natural orbitals for chemical valence (ETS-NOCV). Charge transfer between CT and $C_{20}$ nano-cage were clarified by the charge decomposition analysis (CDA) method.

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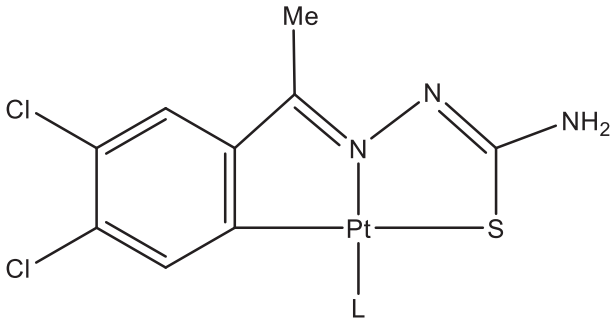



L=$PPh_3$ and 1,3,5-triaza-7-phosphaadamantane

Fig. 1. Structure of two synthesized cycloplatinated thiosemicarbazone complex.

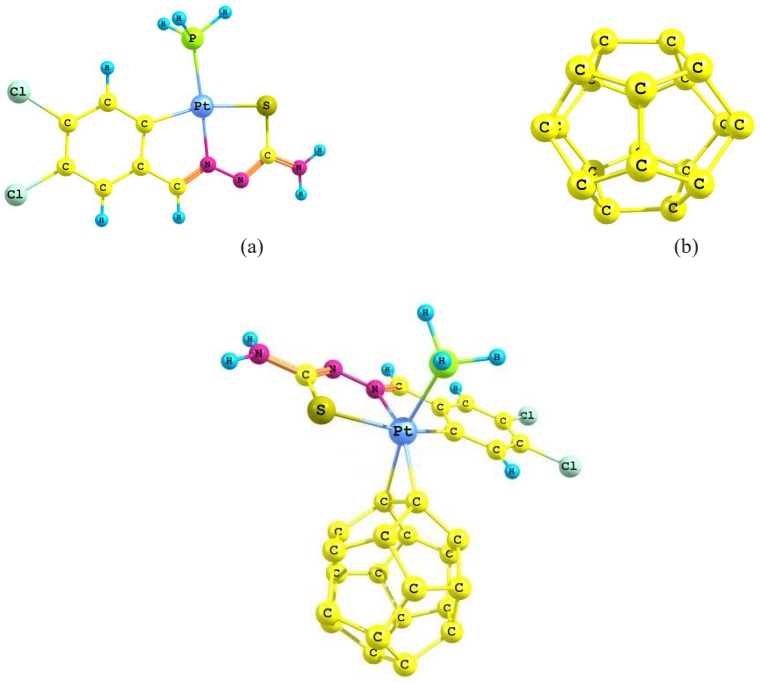



Fig. 2. Structures of (a) studied cycloplatinated thiosemicarbazone complex, (b) $C_{20}$ nano-cage and (c) optimized structure of studied cycloplatinated thiosemicarbazone (CT) with $C_{20}$ nano-cage in gas phase.

## COMPUTATIONAL METHODS

The studied molecules were optimized using software package of Gaussian 09 [45]. The 6-311G (d, p) [46-49] and the Def2-TZVPPD [50] basis sets were considered for the main group elements and Pt element, respectively. Pseudo-potential effective core potential (ECP) was considered for Pt [51]. The Long range-corrected version of wPBE hybrid function (LC-wPBE) was employed [52-55]. Vibrational analysis conformed that optimized molecules were placed on the minimum potential energy curve. Solution phase calculations were done with Self-consistent reaction field (SCRF) method applying the polarizable continuum model (PCM) [56].

Extended Transition State-Natural Orbitals for Chemical Valence (ETS-NOCV), Independent gradient model (IGMH) analysis [57] and Charge

Table 1. Energy (E, a.u), dipole moment (μ, Debye), solvation energy ($\Delta E_{solv}$, kcal/mol) and interaction energy ($\Delta E_{int}$, kcal/mol) of the complex of studied cycloplatinated thiosemicarbazone (CT) with $C_{20}$ nano-cage in gas and solution phases. ε and n are dielectric constant and refractivity index of solvent, respectively.

| | ε | n | E | μ | $\Delta E_{solv}$ | $\Delta E_{int}$ |
|---|---|---|---|---|---|---|
| Gas | - | | -3013.666 | 8.82 | 0.00 | -98.52 |
| CF | 4.71 | 1.45 | -3013.679 | 11.92 | -8.14 | -97.24 |
| DCE | 10.13 | 1.41 | -3013.682 | 12.78 | -10.09 | -96.86 |
| AC | 20.49 | 1.36 | -3013.684 | 13.25 | -11.08 | -96.69 |
| PN | 29.32 | 1.366 | -3013.684 | 13.40 | -11.39 | -96.63 |
| DMF | 37.22 | 1.43 | -3013.684 | 13.47 | -11.55 | -96.61 |
| DMSO | 46.83 | 1.48 | -3013.684 | 13.54 | -11.67 | -96.58 |

decomposition analysis (CDA) [58] were done with Multiwfn 3.8 software package [59]. VMD software was employed to the visualizations of the IGMH result [60].

## RESULTS AND DISCUSSION

*Energetic aspects*

Optimized geometries of $C_{20}$ molecule, CT complex and CT…$C_{20}$ complex are indicated in Fig. 2(a, b, c). Computed energy (E) and solvation energy ($DE_{solv}$) values of CT…$C_{20}$ complex are listed in Table 1. The CT…$C_{20}$ complex in solution phase has larger stability than gas phase and can be found in the basis of E values. There is more significance stability in more polar solvents. It can be found, smaller $DE_{sol}$ values for more polar solvents. Linear relation between dielectric constant of solvents (e) and $DE_{sol}$ data is:

$DE_{sol}$ = -0.0723 e - 8.8628; $R^2$ = 0.7362

Considered solvents are: Propanonitrile (PN), chloroform (DF), acetone (AC), dichloroethane (DCE), n,n-dimethylformamide (DMF), and dimethylsulfoxide (DMSO)

Then, the *modified-Buckingham* function ($F_{modified\text{-}Buckingham}$) [61] is considered as equation follow:

$$F_{modified\text{-}Buckingham}=C_1+C_2.f(\varepsilon)+C_3.f(n^2)+C_4.f(\varepsilon).f(n_2)$$

$$f(\varepsilon)=\frac{(\varepsilon-1)}{2\varepsilon+1};\ f(n^2)=\frac{(n^2-1)}{2n^2+1}$$

This equation includes the influence of solvent dipolarity (f(e)) and solvent polarizability ($f(n^2)$). Third cross-term considers a mutual relationship in polarizability/dipolarity variations due to formed solvent/ solute collision complexes in solution.

The relationship between $DE_{sol}$ values and this solvent polarity function is:

$$\Delta E_{sol}=12.18\text{-}49.47\ f(\varepsilon)\text{-}49.88f(n^2)+ 103.98\ f(\varepsilon).f(n^2);\ R^2=0.9999$$

Therefore, it can be found a good correlation between the $DE_{sol}$ values with *modified-Buckingham* function in the studied system.

*Interaction energy values*

The calculated interaction energy values of the CT…$C_{20}$ complexes are gathered in Table 1. It can be deduced significance interactions between CT and $C_{20}$ nano-cage in solution phase than gas phase. Furthermore, the stronger interaction is observed in more polar solvents. Linear dependence between $DE_{int}$ and e values is:

$DE_{int}$ = 0.0133 e - 97.098; $R^2$ = 0.7164

The relationship between $DE_{int}$ values and the *modified-Buckingham* function is:

$$\Delta E_{int}=\text{-}97.94+2.73f(\varepsilon)\text{-}5.39f(n^2)+11.47\ f(\varepsilon).f(n^2);\ R^2=0.9999$$

It can be observed a significant relation between the values of the $DE_{int}$ values and *modified-Buckingham* function.

*Dipole moment*

Computed dipole moment values of the CT… $C_{20}$ complex are shown in Table 1. It can be deduced higher m values in solution phase than gas phase. Calculated m values are higher in more polar solvents.

Table 2. $\nu_{sym}$(NH) and $\nu_{asym}$(NH) values ($cm^{-1}$) of the complex of studied cycloplatinated thiosemicarbazone with $C_{20}$ nano-cage in gas and solution phases.

| | $\upsilon(N\text{-}H)_{sym}$ | $\upsilon(N\text{-}H)_{asym}$ |
|---|---|---|
| | 3503.00 | 3635.71 |
| Gas | 3663.52 | 3796.41 |
| CF | 3655.47 | 3785.68 |
| DCE | 3654.18 | 3784.39 |
| AC | 3653.48 | 3783.72 |
| PN | 3653.29 | 3783.55 |
| DMF | 3653.21 | 3783.47 |
| DMSO | 3653.16 | 3783.43 |

Linear dependence of the values of e and m values is:

$m = 0.0335\ e + 12.228$; $R^2 = 0.7523$

The relationship between solvent polarity function and m is:

$$\mu = -1.99 + 32.22\ f(\varepsilon) + 44.68\ f(n^2) - 92.99\ f(\varepsilon).f(n^2);\ R^2 = 0.9999$$

Thus, it can be seen good relationship between the m with *modified-Buckingham* function in the studied system.

*Vibrational spectrum analysis*

The vibrational analysis of CT…$C_{20}$ complexes reveal that that the maximum wavenumber values of this complex is due to the asymmetric and symmetric stretching vibration modes of amine ligands. Computed $n_{sym}$(NH) and $n_{asym}$(NH) values are gathered in Table 2. These values are larger in solution phase than gas phase. Larger values are found in less polar solvents.

The induced stretching frequency shifts was provided by *modified-Buckingham* function as follows:

$$\frac{(\upsilon_{solution} - \nu_{gas})}{\nu_{gas}} = \frac{\Delta\upsilon}{\nu_{gas}} = C_1 + C_2.f(\varepsilon) + C_3.f(n^2) + C_4.f(\varepsilon).f(n^2)$$

It can be provided good linear correlation between solvent-induced stretching vibrational frequency shifts of u(NH) with the *modified-Buckingham* function:

$$\Delta\upsilon/\nu_{gas} = 1.75 \times 10^{-3} - 9.68 \times 10^{-3}\ f(\varepsilon) - 1.03 \times 10^{-2}\ f(n^2) + 2.24 \times 10^{-2}\ f(\varepsilon).f(n^2);\ R^2 = 0.9999$$

*Molecular orbital analysis*

Plots of frontier orbitals of the $C_{20}$…CT complexes are presented in Fig. 3 in the gas phase. It can be deduced, $C_{20}$ fragment includes most contributions in HOMO and LUMO. Comparison of the frontier orbital energy values in the CT and $C_{20}$…CT complex indicates CT interaction with $C_{20}$ importantly destabilizes and stabilizes the HOMO and LUMO levels of CT, respectively. In addition, HOMO-LUMO gap value is larger in $C_{20}$…CT complex than CT. Therefore, we believe that the $C_{20}$ may be a suitable nanoscale carrier for CT drug.

*ETS-NOCV method*

The Extended Transition State - Natural Orbitals for Chemical Valence (ETS-NOCV) method [62] is defined a mixture of the NOCV method [63] and the ETS approach [64].

ETS-NOCV outcomes reveal that NOCV pair 1 is the main contributor to the D$E_{orb}$ (-328.25 kcal/mol). Computed NOCV pair 1 energy value is -161.94 kcal/mol. The Fig. 4 displays the isosurface of NOCV pair density pair 1. Enhanced and reduced and the electron density are presented with green and blue isosurfaces, respectively, owing to the orbital interaction defined by NOCV pair 1. Obviously, the NOCV pair 1 attributes to important electron shift from the CT fragment to the $C_{20}$ nano-cage. 1.05482 electron is moved electron to this NOCV pair.

*IGMH analysis*

The interaction of CT…$C_{20}$ is evaluated with independent gradient model (IGM) based on Hirshfeld partition of molecular density (IGMH) (Fig. 5). It can be detected the Pt..C interactions

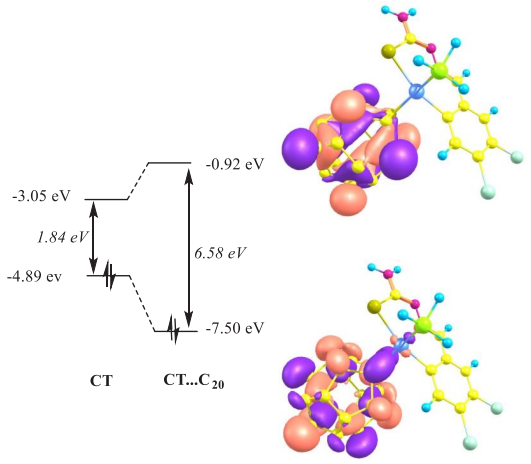



Fig. 3. Plots of frontier orbitals C20…CT complex in gas phase.

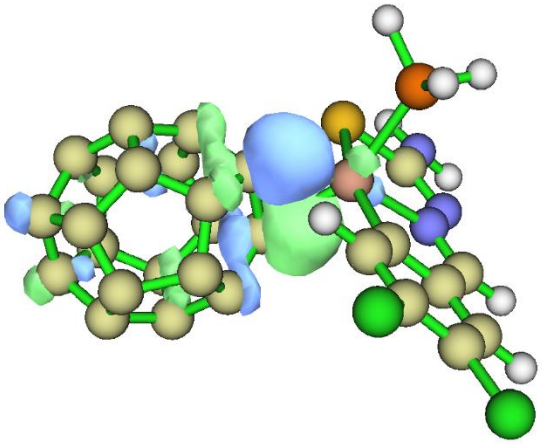


Fig. 4. Isosurface of NOCV pair density pair 1 of CT…$C_{20}$ complex.

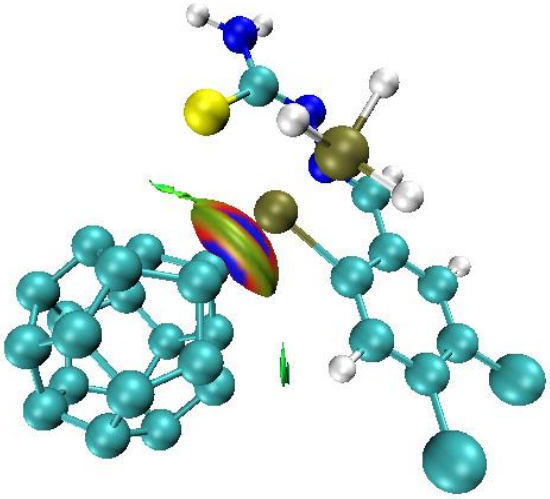


Fig. 5. Independent gradient model (IGM) based on Hirshfeld partition of molecular density (IGMH) of CT…$C_{20}$ complex.

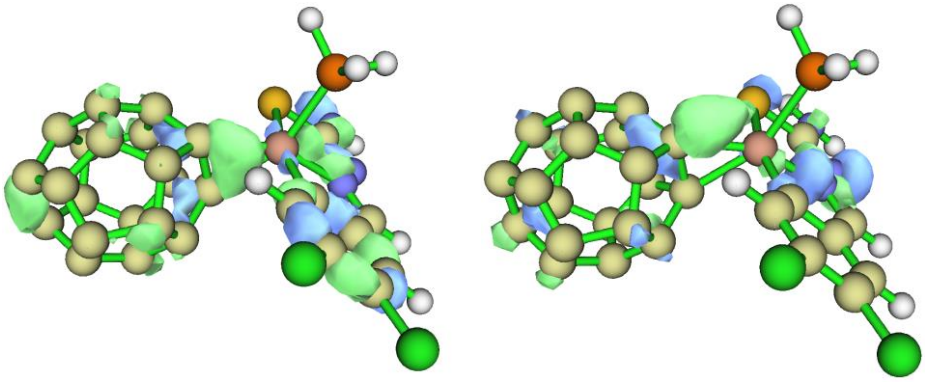
(blue color), nearby the middle of the isosurface.

*CDA*

The charge decomposition analysis (CDA) theory is beneficial approaches to afford significant intuition into the electron transfer. The CDA outcomes display orbital 131 leads 0.017229 electrons donate from $C_{20}$ cage to CT complex. On the other hand, 0.021980 electrons detached from overlap area between $C_{20}$ cage and CT. Orbital 88 has small contribution to electron donation (0.037670 electron). Fig. 6 displays isosurfaces of orbital 88 and 131. Also, extended charge decomposition analysis (ECDA) shows that 0.5875 electrons moved from fragment CT complex to $C_{20}$ cage.

**CONCLUSION**

In this work, we reported the interaction of a cycloplatinated thiosemicarbazone (CT) as antitumor and antiparasitic agents with $C_{20}$ molecule. Our calculations revealed the CT…$C_{20}$ interaction increases in solution than gas phase. The more significance interaction was found in more polar solvents. Smaller polarity was deduced in gas phase than solution phase. The vibrational analysis revealed the maximum wavenumber values of the investigated complex were belonged to the asymmetric and symmetric stretching vibration modes of amine ligands (u(N-H)). Significance relationships were provided between m, $DE_{solv}$, $DE_{int}$ and u(N-H) data with *modified-Buckingham* function in the CT…$C_{20}$ systems. ETS-



**88** **131**

Fig. 6. Isosurfaces of orbitals 88 and 131 of CT…$C_{20}$ complex.

NOCV outcomes illustrated NOCV pair 1 was the highest subscriber to the D$E_{orb}$ (-328.25 kcal/mol). NOCV pair 1 energy value of the CT…$C_{20}$ system was -161.94 kcal/mol. CDA findings illustrated electrons donate from CT complex to $C_{20}$ molecule.

## CONFLICTS OF INTEREST

The authors do not have any conflicts of interest.

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