

DFT Study of Benzamide Coordination with Zinc (II)

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Authors' contributions

Author UAK designed the study, performed the calculations and wrote the first draft. Author GSYA performed a part of calculations and helped to analyse the results. Authors AGK and ATKH helped to analyse the results. Author LAB allowed LaC The SMO (Laboratory of Theoretical Chemistry and Molecular Spectroscopy) research team to perform some calculations on the server of his laboratory. Author JBM is LaC The SMO Director; he managed this scientific work. All authors read and approved the final manuscript.

Original Research Article

Received 31st October 2013
Accepted 28th January 2014
Published 20th February 2014

ABSTRACT

Benzamide ($C_6H_5CONH_2$) is the first representative of the aromatic acid amides. Its molecule contains an amide group. Amide group is the main structural unit of polyamides, peptides and proteins. This functional group plays a special role in very important vital processes. The aromatic acid amides and their derivatives, as well as other amides, are widely used in medicine as physiologically active substances, as the central nervous system stimulants, and as antituberculosis substances. The coordination of these compounds profoundly modifies the physiological properties of metals and those of ligands in the direction of the overall positive modification of these properties. Benzamide, like other amides, contains two donor atoms (nitrogen and oxygen). It is important to know the potential donor that takes part in the coordination bond. To answer these questions we referred to quantum methods. We performed the calculations by the DFT/B3LYP method in the Lanl2dz basis set using the Gaussian 98W program on the

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computer HPL1908w. First we studied the benzamide molecule and then we simulated its complexation with $ZnCl_2$. From the analysis of the results which take into account the atomic charges, atom electrostatic potentials and other energy parameters of the studied systems, it appears that the coordination bond of benzene with zinc takes place via the oxygen atom; and the complex obtained was the dichloro di benzamide zinc (II) complex which formula was $[Zn (C_6H_5CONH_2)_2Cl_2]$.

Keywords: Benzamide; zinc (II) chloride; nitrogen; oxygen; dichloro di benzamide zinc (II); DFT/B3LYP; lanl2dz.

1. INTRODUCTION

Amide group is the main structural unit of polyamides, peptides and proteins. This functional group plays a special role in the vital processes. Several drugs and bio-stimulators contain the amide group. For example, one finds the amide group in nicotinamide (vitamin B₃) and in the cordiamine which are very valuable drugs. The aromatic acid amides and their derivatives, as well as other amides, are widely used in medicine as physiologically active substances, as central nervous system stimulants, and as antituberculosis substances.

The study, at the molecular level, of the interaction between metals and bioligands (proteins, nucleic acids, and other bio-substances) is topical [1-3]. The coordination of these compounds profoundly modifies the physiological properties of metals and those of ligands in the direction of the overall positive modification of these properties. The bioinorganic chemistry is studying ardently the coordination of trace elements with amides [4-7]. Benzamide, like other amides, contains two pair donor atoms (nitrogen and oxygen). It is important to know the potential pair donor that takes part in the coordination. To answer these questions the use of quantum methods is indicated. The functional density theory (DFT) is, in this twenty-first century, one of the most used methods in quantum calculations of the system electronic structure. This is the method we used in the present work which is devoted to the study of the benzamide reactivity as a ligand.

2. MATERIALS AND METHODS

2.1 Theory and Software Used

In this work the calculations were made by the use of DFT method assisted by B3LYP. Traditional methods in the theory of electronic structure of the element (HF and derived methods from this formalism) are based on a function of multielectronic wave of matter. The main objective of DFT is to replace the multielectronic wave function by electron density. While the multielectronic wave function depends on $3N$ variables (where N is the total number of particles in the system), the density is only a function of three variables; this is easier to handle mathematically and conceptually. The principle of DFT is a reformulation of a quantum many-body problem in a unibody problem, or at most, bibody considering issues spin. The central idea of the DFT is: only the ground state electron density of the system completely determines the main observables values [8,9]. The density functional method is a self-consistent method which converges cycles.

The total density is calculated from a Slater determinant, which requires a suitable atomic orbital basis. B3LYP functional is the most used by chemists. This symbol means that the

energy exchange is calculated by the use of Becke's method with three parameters and the correlation by the method of Lee, Yang and Parr [10-12]. DFT methods is close to MP2 by quality; also DFT computation time is lower than that of MP2, so that method proved better than MP2 for many systems [9]. This is precisely the DFT/B3LYP method we have chosen essentially for investigation in the present work. We used essentially the software Gaussian 98 and 03 [13].

This work was carried out at the "Laboratoire de chimie Théorique et de Spectroscopie Moléculaire" of "Université d'Abomey-Calavi", Benin and on the server of the Department of Chemistry, Rutgers University United States.

2.2 Modeling of the Reaction

The present study contains the following three stages:

- 1 Optimization of reagents (zinc (II) chloride and benzamide). At this stage we attempted to define the probable coordination site in the benzamide molecule.
- 2 Phased approach of one molecule of $ZnCl_2$ to one benzamide molecule with the aim to ascertain the most stable complex conformer formed from benzamide and zinc (II) chloride.
- 3 Progressive approach of one molecule of the $[ZnCl_2\text{-benzamide}]$ complex to one benzamide molecule in the aim to obtain a complex according to the usual coordination number of zinc (II).

At each stage of the study we analyzed various system parameters, such as geometric data, atomic charges, molecular electrostatic potentials and the frontier orbitals.

3. RESULTS AND DISCUSSION

3.1 The Benzamide

3.1.1 Analysis of geometric parameters

The optimized structure of the benzamide molecule is shown on Fig. 1.

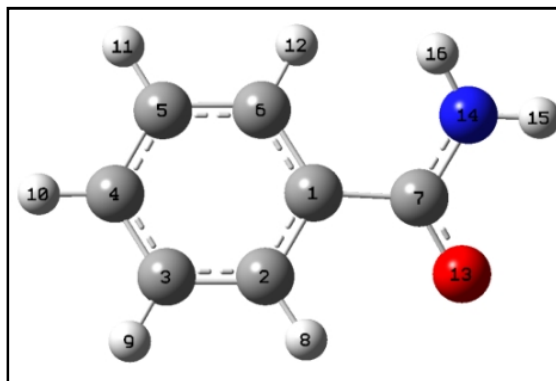


Fig. 1. Benzamide molecule Structure

Table 1 summarizes some geometric parameters of the benzamide molecule.

In this molecule the aromatic ring makes an angle of about 15° with the plane of the amide group; this means that the benzamide molecule is not flat. This observation is consistent with experimental data [14,15]. Rotation of the amide group relative to the aromatic ring might result from the repulsion interaction between the hydrogen atoms of the amide group and those of the aromatic ring.

Table 1. Geometric parameters of the benzamide molecule

Bonds	C=O	C-N	N-H	N-H	C ₁ -C ₇
Lengths (Å)	1.26	1.381	1.012	1.01	1.506
Angles	$\alpha_{(OCN)}$	$\alpha_{(NCC)}$	$\alpha_{(C7NH15)}$	$\alpha_{(C7NH16)}$	$\alpha_{(H15NH16)}$
Values (°)	120.90	117.28	117.62	123.10	119.01
Dihedrals	$\tau_{(OC7C1C2)}$	$\tau_{(OC7C1C6)}$			
Values (°)	15.670	-163.43			

The sum of the angles around N atom is close to 360°, which means that the nitrogen is in sp^2 hybridization state.

In this case the non-bonding electron pair of the nitrogen atom has a p almost pure character so the corresponding electron cloud is oriented perpendicularly to the NC⁷O plan. This orientation is favorable to the interaction of this free electron cloud and the π electrons of the CO bond: conjugation effect is then possible and does not lead to the coordination of benzamide molecule through the nitrogen atom.

The analysis of the bond lengths reveals that the length of C = O bond (1.26 Å) is greater than the standard length (1.20 Å), the length of the C-N (1.38 Å) bond is less than the standard length (1.47 Å) [16,17]; in other words it can be said that these calculated bond length values are intermediate between the double bonds and single bonds. This confirms that the π electrons of the CO bond are combined with the p lone pair of the nitrogen atom, which is in good agreement with the literature data [18]. C₁-C₇ bond \approx 1.51 Å is slightly short; this is probably the result of a conjugation between the aromatic ring and the amide fragment.

3.1.2 Analysis of atomic charges

The charge analysis of Mulliken population was carried out in the present work Table 2.

Table 2. Physic: Some Mulliken atomic charges in the benzamide molecule

Atoms	O	N	H ¹⁵	H ¹⁶	C ¹	C ⁷
Charges (ua)	-0.3092	-0.6432	0.3369	0.318	0.3033	0.1726

The Table 2 shows that the electron density at the nitrogen atom is higher than that at the oxygen atom. This observation implies that coordination through the nitrogen atom is much more likely as through the oxygen atom, however the nitrogen atom environment is not favorable to this attack: it is surrounded by three atoms (H¹⁵, H¹⁶ and C⁷) with large positive charges, which are able to repel the Zn (II). The benzamide molecule reactivity was also discussed considering the electrostatic potential around atoms. Table 3 summarizes the significant atomic electrostatic potentials of the benzamide molecule.

3.1.3 Analysis of electrostatic potentials

From the analysis of the Table 3, we notice that the electrostatic potential at the level of the oxygen atom is higher than that at the nitrogen atom's. This suggests that the benzamide, at the time of the coordination, goes into the coordination sphere through the oxygen atom.

Table 3. Electrostatic potentials at the level of some atoms in the benzamide molecule

Atoms	O	N	H ¹⁵	H ¹⁶	C ¹	C ⁷
Electrostatic potentials (ua)	-22.381	-18.3493	-0.9981	-0.99	-14.730	-14.634

3.1.4 Partial conclusion

The three coordination criteria (geometric data, atomic charges, molecular electrostatic potentials) which was considered in this study suggest that the coordination of the benzamide molecule occurs via the oxygen atom. Now it is important to simulate the reaction of benzamide complex formation in the aim:

1. To confirm this result,
2. To define the most stable conformer; indeed, given that both free electron pairs at the O¹³ atom are respectively in cis and trans positions relative to the nitrogen atom, the formation of two complexes which would be conformational isomers is possible; then it is suitable to define the most stable conformer.

3.2 The Benzamide.ZnCl₂ Complex

It should be reminded that the electronic structure of zinc (II) is $1s^2 2s^2 2p^6 3s^2 3p^6 4s^0 3d^{10} 4p^0$. The highest occupied molecular orbitals (HOMO) and the lowest unoccupied molecular orbitals (LUMO) were examined. We have noticed that the difference between benzamide's HOMO (-0.255 hartree) and the LUMO (-0.1124 hartree) of ZnCl₂ is 0.14 hartree. This is smaller than the difference between the HOMO of Zinc chloride (-0.324 hartree) and benzamide's LUMO (-0.0509 hartree) whose value is 0.27 hartree. This observation allows envisaging the complexation reaction where the benzamide molecule serves as electron pair donor and the ZnCl₂ molecule would be the acceptor [19]. Note that the LUMO of ZnCl₂ is dominated by the s orbital, and the HOMO of benzamide by the p_x orbital.

The structure of the studied system is shown in Fig. 2. Table 4 shows the parameters of the system at the beginning and the end of the reaction. The reaction was led at 100°C and 1 atm according to a previous experimental investigation [18].

The simulation of this process has consisted in moving ZnCl₂ near to Benzamide, starting with the distance ZnO = 3 Å. At the same time the distance ZnN was almost 3 Å too. The temperature of the system was 100°C according to prior experimental study [18]. The end of the coordination process was obtained in a total relaxation of the system.

Geometric and energetic parameters varied during the reaction. In the end, the ZnO distance was 1.99 Å while ZnN was equal to 3.49 Å. These data show that the coordination bond was formed through the oxygen atom [18,19] and not through the nitrogen atom.

We can therefore conclude that the value of the electrostatic potential at the level of the atoms is a good criterion for predicting the coordination site of the metal ions on the ligands. The HOMO value of the coordination product was -0.274 hartree; this value is lower than that of the donor HOMO and is lower than that of the acceptor's LUMO. This situation is in perfect agreement with the theory of molecular orbital formation [16,19,21] and confirms the formation of complex.

Table 4. Parameters of the system at the beginning and the end of the reaction.

Paramters	Beginning of the reaction	End of the réaction
Distances (Å)		
C ⁷ N ¹⁴	1.381	1.35
C ⁷ O ¹³	1.26	1.291
Zn ¹⁷ N ¹⁴	4.063	3.487
Zn ¹⁷ O ¹³	3.000	1.995
Angles (°)		
N ¹⁴ C ⁷ O ¹³	120.90	120.58
N ¹⁴ C ⁷ C ¹	117.28	120.55
O ¹³ C ⁷ C ¹	121.81	118.86
Zn ¹⁷ N ¹⁴ C ⁷	74.878	61.807
Zn ¹⁷ O ¹³ C ⁷	129.49	139.0
Cl ¹⁸ Zn ¹⁷ Cl ¹⁹	180	138.83
Cl ¹⁸ Zn ¹⁷ O ¹³	-	103.55
O ¹³ Zn ¹⁷ Cl ¹⁹	-	117.62
Dihedrals (°)		
N ¹⁴ C ⁷ C ¹ C ²	-163.79	170.52
O ¹³ C ⁷ C ¹ C ²	15.670	-9.118
Zn ¹⁷ O ¹³ C ⁷ C ¹	-179.93	-179.94
Zn ¹⁷ O ¹³ C ⁷ N ¹⁴	-0.4761	0.417
Cl ¹⁸ Zn ¹⁷ O ¹³ Cl ¹⁹	-	179.50
Charges (ua)		
N ¹⁴	-0.643	-0.614
O ¹³	-0.309	-0.513
Zn ¹⁷	0.592	0.730
Energies (hartree)		
HOMO _{BA} *	-0.255	-
LUMO _{BA}	-0.0509	-
HOMO _{ZnCl2}	-0.324	-
LUMO _{ZnCl2}	-0.1124	-
HOMO _{Zn(BA)Cl2}	-	-0.274
LUMO _{Zn(BA)Cl2}	-	-0.01
Enthalpy _(100°C)	-496.334	-496.392
Gibbs energy _(100°C)	-496.433	-496.470

*BA = Benzamide

During the coordination process C⁷N¹⁴ bond has undergone a considerable shortening (length is increased from 1.38 Å to 1.35 Å) while the C⁷O¹³ bond underwent reverse deformation from 1.26 Å to 1291 Å. This observation tells that the binding of zinc on oxygen caused an electron deficit in the oxygen atom, which weakens the C⁷O¹³ double bond; at the same time a strengthening of the nitrogen's p electron delocalization was made to compensate somewhat for the loss of electron density of the O¹³ atom.

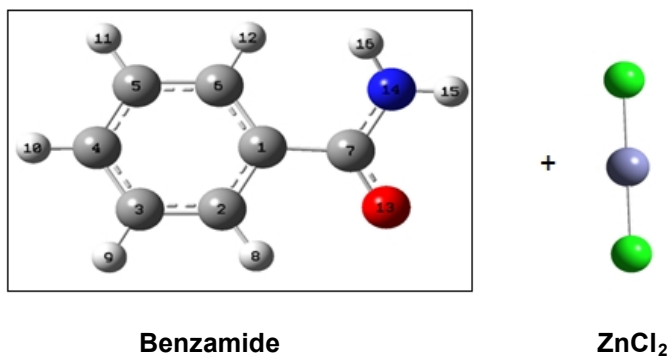


Fig. 2. Structure of the reagents

Considering the values of the dihedrals we noticed that the zinc (II) is fixed in the cis position relative to the N¹⁴ atom at the time of the coordination. The respective values of the free energies of the complex's cis conformation (-496.470 au) and of the complex's trans conformation (-496.449 au) confirms that the cis conformation obtained spontaneously in the present work is the most stable. So it is the dominant conformation.

The value of about 180° of the Cl¹⁸Zn¹⁷O¹³Cl¹⁹ dihedral indicates that these four atoms are in the same plan. The sum of the angles around the zinc atom is equal to 360°, suggesting that the Zn atom in the Zn(Benzamide)Cl₂ complex is in the sp² hybridization state. In this way this complex is a triangle, summits of which are occupied by the two Cl atoms and the oxygen atom O¹³; this figure corresponds to the coordination number 3 that the zinc (II) in this compound has Fig. 3.

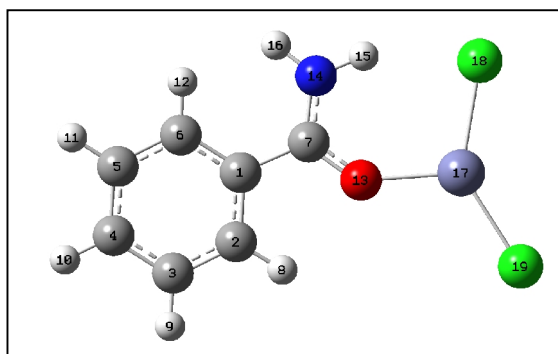


Fig. 3. Structure of the formed complex (The chloro di benzamide zinc (II))

However, this coordination number is not the most stable for zinc (II). According to data from the literature, one attributes the coordination number 4 to the zinc (II) usually [19-27]; as well as the experimental studies [18] had led to the synthesis of Zn(benzamide)₂Cl₂ from an equimolar mixture of ZnCl₂ and of benzamide. All these considerations had led to simulate the formation reaction of the coordination compound Zn(Benzamide)₂Cl₂.

3.3 The (Benzamide)₂. ZnCl₂ Complex

We simulated the formation of Zn(Benzamide)₂Cl₂ approaching one Benzamide molecule to one Zn(Benzamide)Cl₂ molecule Fig. 4.

The simulation of the fixing process of a second molecule of benzamide on Zinc (II) chloride was to approach progressively the two reactants from the distance ZnO²⁰ = 3 Å. The end of the process was obtained in a total relaxation of the system.

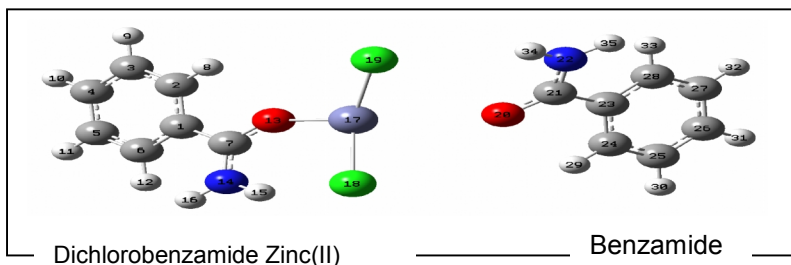


Fig. 4. Structure of the reagents

At the end of the process the Zn¹⁷O²⁰ distance took the value 2.029 Å, which corresponds to the formation of a Zn-O bond. Both Zn-O bonds are equivalent since they are the same length. Immediate environments of zinc (II) in the three directions of space are four (4): two oxygen atoms, each contained in a molecule of the benzamide and two Cl-ions (Zn-O=2.029 Å, Zn-Cl = 2.340 Å), which means that the coordination number of zinc in the complex compound formed from one molecule of ZnCl₂ and two molecules of benzamide is 4, what is a tetrahedron; zinc is here in a sp³ hybridization state. The four ligands occupy each a vertex of the tetrahedron and zinc occupies the tetrahedron center: O¹³ and O²⁰ occupy two opposite vertices, Cl¹⁸⁽⁻⁾ and Cl¹⁹⁽⁻⁾ are on the other two opposite vertices. The lengths of Zn-O and Zn-Cl bonds are different. In that way one can declare that the tetrahedron formed by this compound is irregular. The various geometrical parameters Table 5 confirm this observation. The result of the reaction is shown in Fig. 5. This is the complex dichlorodibenzamide zinc (II) with the formula Zn (C₆H₅CONH₂)₂Cl₂ or Zn(Benzamide)₂Cl₂. The Zn¹⁷O¹³C⁷N¹⁴ and Zn¹⁷O²⁰C²¹N²² dihedrals value was -5.1°. That confirms that the zinc was in the cis position relative to each of the two amidic nitrogen atoms.

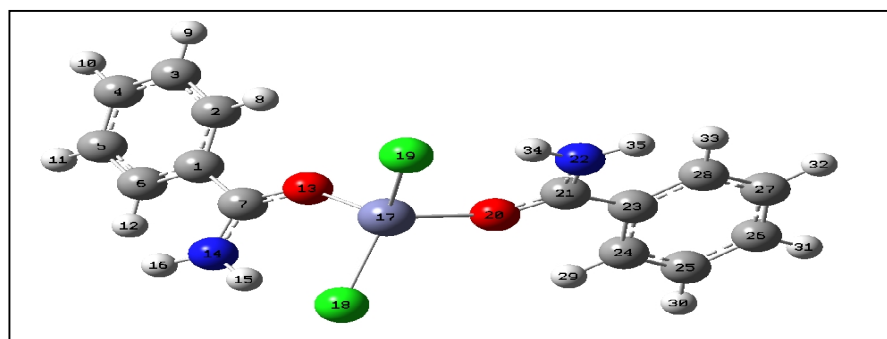


Fig 5. Structure of the reaction product, the dichlorobenzamide zinc (II)

Table 5. Parameters of the system at the beginning and the end of the reaction

Parameters	Beginning of the reaction 2 ⁽¹⁾	End of the reaction 2
Distances (Å)		
C ⁷ N ¹⁴	1.35	1.352
C ⁷ O ¹³	1.291	1.284
Zn ¹⁷ N ¹⁴	3.487	3.489
Zn ¹⁷ O ¹³	1.995	2.029
C ²¹ N ²²	1.381	1.352
C ²¹ O ²⁰	1.26	1.284
Zn ¹⁷ N ²²	4.063	3.489
Zn ¹⁷ O ²⁰	3.000	2.029
Angles (°)		
N ¹⁴ C ⁷ O ¹³	120.58	121.21
N ¹⁴ C ⁷ C ¹	120.55	119.68
O ¹³ C ⁷ C ¹	118.86	119.11
Zn ¹⁷ N ¹⁴ C ⁷	61.807	62.262
Zn ¹⁷ O ¹³ C ⁷	139.0	137.47
Cl ¹⁸ Zn ¹⁷ Cl ¹⁹	138.83	125.90
Cl ¹⁸ Zn ¹⁷ O ¹³	103.55	102.54
O ¹³ Zn ¹⁷ Cl ¹⁹	117.62	110.86
N ²² C ²¹ O ²⁰	120.90	121.21
N ²² C ²¹ C ²³	117.28	119.68
O ²⁰ C ²¹ C ²³	121.81	119.11
Zn ¹⁷ N ²² C ²¹	74.878	62.262
Zn ¹⁷ O ²⁰ C ²¹	129.49	137.47
Cl ¹⁸ Zn ¹⁷ O ²⁰	-	110.84
O ²⁰ Zn ¹⁷ Cl ¹⁹	-	102.55
Dihedrals (°)		
N ¹⁴ C ⁷ C ¹ C ²	170.52	161.86
O ¹³ C ⁷ C ¹ C ²	-9.118	-17.59
Zn ¹⁷ O ¹³ C ⁷ C ¹	-179.94	174.35
Zn ¹⁷ O ¹³ C ⁷ N ¹⁴	0.417	-5.083
Cl ¹⁸ Zn ¹⁷ O ¹³ Cl ¹⁹	179.50	136.69
N ²² C ²¹ C ²³ C ²⁴	-163.79	161.76
O ²⁰ C ²¹ C ²³ C ²⁴	15.670	-17.68
Zn ¹⁷ O ²⁰ C ²¹ C ²³	-179.93	174.32
Zn ¹⁷ O ²⁰ C ²¹ N ²²	-0.4761	-5.11 5
Cl ¹⁸ Zn ¹⁷ O ²⁰ Cl ¹⁹	-	-136.68
Charges (ua)		
N ¹⁴	-0.614	-0.614
O ¹³	-0.513	-0.476
Zn ¹⁷	0.730	0.751
N ²²	-0.643	-0.614
O ²⁸	-0.309	-0.476
Energies (HF)		
HOMO _{Zn(BA)2Cl2}	-	-0.2506
LUMO _{Zn(BA)2Cl2}	-	-0.0076
Enthalpy (100°C)	-897.159	-897.195
Free enthalpy(100°C)	-897.282	-897.306

*BA=benzamide; ΔH_1 and ΔG_1 are enthalpy and free enthalpy of reaction 1, ΔH_2 and ΔG_2 are enthalpy and free enthalpy of reaction 2, ΔH and ΔG are enthalpy and free enthalpy of the sum of reactions 1 and 2

In sum our investigations was a simulation of the reaction between one mole of zinc chloride and two benzamide moles .The reaction is shown in Fig. 6.

The energy balance presented in the Table 6 shows that the coordination of zinc (II) with benzamide is an exothermic process since it evolved as a decrease in enthalpy. The process is spontaneous because its free energy was negative.

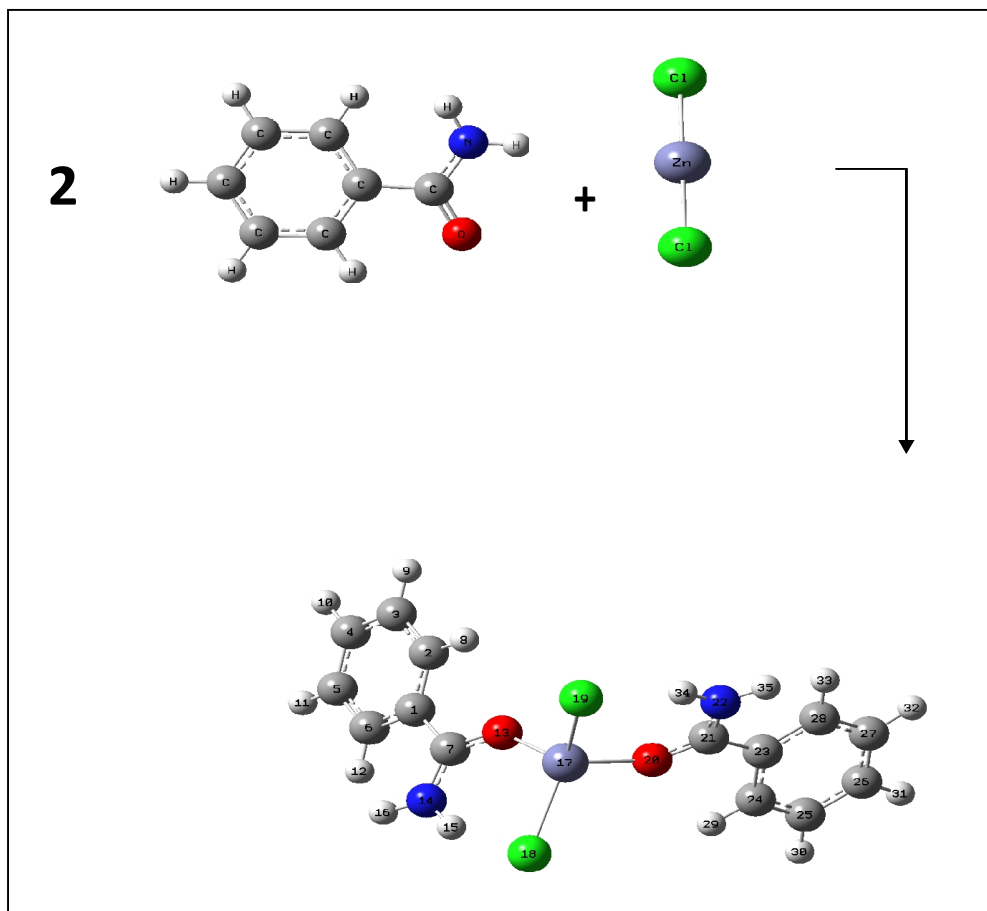


Fig. 6. Scheme of the reaction between 1 mole of $ZnCl_2$ and 2 moles of benzamide: formation of dichlorobenzamide zinc (II)

Table 6. Energy balance of the coordination process of $ZnCl_2$ with benzamide

Enthalpy (ua)				ΔH_1	ΔH_2	$\Delta H(ua)$	
$ZnCl_2$	BA^*	$ZnCl_2BA$	$ZnCl_2(BA)_2$	ua	ua	ua	$kJ.mol^{-1}$
-95.577	-400.757	-496.397	-897.195	-0.063	-0.041	-0.104	-237.052
Free enthalpy (ua)				ΔG_1	ΔG_2	ΔG	
$ZnCl_2$	BA^*	$ZnCl_2BA$	$ZnCl_2(BA)_2$	ua	ua	ua	$kJ.mol^{-1}$
-95.619	-400.813	-496.455	-897.306	-0.023	-0.038	-0.061	-160.155

4. CONCLUSION

The present work focused on the DFT study of coordination of Zinc (II) with benzamide. This study was conducted in three main stages:

The first stage was to study the reactivity of the benzamide molecule as a ligand. Having found that the benzamide molecule has two possible coordination centers namely the nitrogen atom and the oxygen atom of the amide group, we have, under geometrical parameters, atomic charges, electrostatic potentials at atoms, determined that the coordination of the ligand with a metal ion is preferably carried out via the oxygen atom, which is to comply with the literature data. To predict the position of the metal ion on the oxygen, we discussed the second stage of our study.

At the second step we simulated the reaction between a benzamide molecule and a molecule of zinc (II) chloride. It appeared that the zinc by binding to the amide oxygen atom, occupied the cis position relative to the nitrogen atom, so the cis position is most likely in the complexation of benzamide. It follows from this that the formation of the complex dichlorobenzamide zinc (II) is possible. The coordination number of the zinc in this compound was 3. It must be recognized that the coordination number 4 is rather that which characterizes mainly zinc (II). It is for this reason that we considered the model $Zn(BA)_2Cl_2$ where zinc (II) is under the coordination number 4.

The third stage of this work led to the formation of dichlorodibenzamide zinc (II) with the formula $[Zn(BA)_2Cl_2]$, a tetrahedral zinc complex.

This study thus showed that the formation of $[Zn(BA)_2Cl_2]$ from $ZnCl_2$ and BA is possible and confirms our previous experimental results. This process is exothermic and spontaneous since the values of the enthalpy and that of the free enthalpy of the transformation were negatives.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

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