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Density functional calculations of oxygen, nitrogen and hydrogen electric field gradient and chemical shielding tensors to study hydrogen bonding properties of peptide group (O=C–NH) in crystalline acetamide

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Abstract

A density functional theory (DFT) study was carried out to investigate hydrogen bonding (HB) properties of peptide group (O=C–NH) in crystalline acetamide. Since the peptide group in acetamide contributes to N–H···O and C–H···O types of HB interactions, acetamide is considered as the simplest form of peptide linkage in proteins. The evaluated NMR parameters including quadrupole coupling constants and asymmetry parameters from the calculated electric field gradient (EFG) tensors at the sites of O17, N14 and H2 nuclei and isotropic chemical shieldings from the calculated chemical shielding (CS) tensors at the sites of O17, N15 and H1 nuclei reveal the major contribution of O=C–NH group to HB interactions. Although N–H···O type of HB interaction play the major role in the HB properties of peptide group in lattice form of crystalline acetamide, however, the role of weaker C–H···O type of HB interaction cannot be neglected.

Keywords: DFT; NMR; Hydrogen bond; Peptide; Acetamide

1. Introduction

Hydrogen bonding (HB) interactions play unique roles in various living systems, e.g., in determination of the structural properties and also in stabilization of the β-sheets in proteins [1]. Because the macromolecular protein structures are very complex to study, studying the simplest models having the major characteristic of proteins is an advantage in the investigation of HB properties in these structures. Acetamide with a single peptide group (O=C–NH) can be considered as the simplest model system of peptide linkage in proteins and polypeptides. Acetamide is capable of contributing to N–H···O=C and C–H···O=C types of HB interactions which are very important in the stabilization of α-helix and β-sheet structures and numerous studies using various techniques were devoted to characterize the properties of them [2–14].

Since the most characteristic nature of HB is electrostatic, those techniques dealt with this nature are proper in the investigation of HB properties. Among them, nuclear magnetic resonance (NMR) spectroscopy is an important technique to study the properties of various types of HB interactions. Electric field gradient (EFG) and chemical shielding (CS) tensors arisen by the electronic environment at the sites of quadrupole nuclei, e.g., ^{17}O, ^{14}N and ^{2}H, and magnetic nuclei, e.g., ^{17}O, ^{15}N and ^{1}H, respectively, are significantly influenced by HB interactions and are such useful elements to study HB interactions properties in the considered hydrogen bonded systems [15,16].

Present work calculates NMR tensors (EFG and CS) at the sites of oxygen, nitrogen, and hydrogen nuclei to study the properties of HB interactions of the peptide group (O=C–NH) in acetamide. To this aim, the crystalline coordinates of acetamide at 146 K was obtained from X-ray study of Bats et al. [17] and the hydrogen bonded six-molecule lattice consisting of those the most possible HB interacting molecules through N–H···O and C–H···O HB types was created by coordinates transforming (see Table 1 and Fig. 1). To systematically

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Table 1
The geometrical properties of acetamide

Intramolecular	Before H-optimization[a]	After H-optimization[b]
*r*N–H1	0.90 Å	1.01 Å
*r*N–H2	0.87 Å	1.02 Å
*r*C1–O	1.24 Å	1.24 Å
*r*C2–H	0.98 Å	1.09 Å
Intermolecular		
*r*N···O [No. 3]	2.93 Å	2.93 Å
*r*N···O [No. 2]	2.87 Å	2.87 Å
*r*N–H1···O [No. 3]	2.03 Å	1.94 Å
*r*N–H2···O [No. 2]	2.01 Å	1.86 Å
*r*O···N [No. 3]	2.99 Å	2.99 Å
*r*O···C2 [No. 4]	3.47 Å	3.47 Å
*r*O···N [No. 5]	2.87 Å	2.87 Å
*r*O···H1–N [No. 3]	2.05 Å	1.90 Å
*r*O···H–C2 [No. 4]	2.49 Å	2.37 Å
*r*O···H2–N [No. 5]	2.01 Å	1.86 Å
*r*C2···O [No. 6]	3.47 Å	3.47 Å
*r*C2–H···O [No. 6]	2.49 Å	2.37 Å
∠N–H1···O [No. 3]	117.6°	162.6°
∠N–H2···O [No. 2]	168.1°	168.3°
∠O···H1–N [No. 3]	171.6°	169.4°
∠O···H–C2 [No. 4]	177.8°	176.4°
∠O···H2–N [No. 5]	168.1°	163.8°
∠C2–H···O [No. 6]	177.7°	177.8°

See Fig. 1 for details.
[a] The original coordinates from reference [17] are considered.
[b] The H positions of original coordinates are just optimized.

investigate the HB properties of O=C–NH group in the considered system, the NMR tensors were calculated for acetamide in its monomer, a representative dimer and lattice crystalline forms. Table 2 presents the quadrupole coupling constants (C_Q) and asymmetry parameters (η_Q) evaluated by the calculated EFG tensors at the sites of ^{17}O, ^{14}N and ^{2}H nuclei and Table 3 presents the isotropic chemical shieldings (σ_{iso})

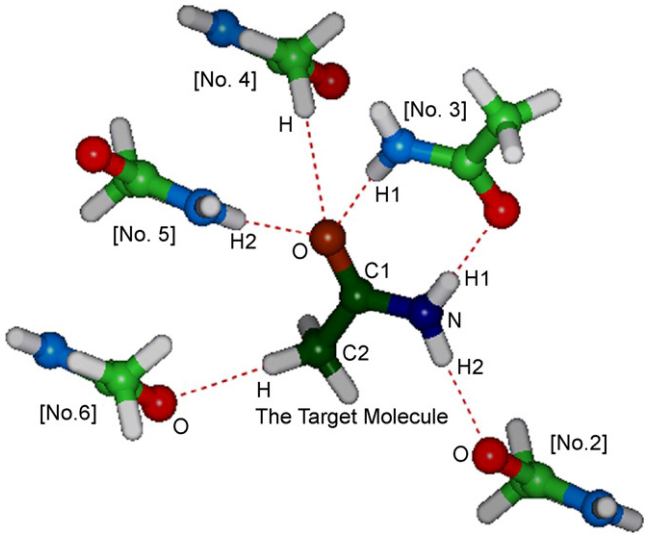

Fig. 1. The six-molecule lattice of crystalline acetamide. In monomer model, just the target molecule and in dimer model, the target molecule and molecule [No. 3] are considered. Dash lines show HB interactions (see Table 1 for details).

Table 2
The EFG tensors at the sites of ^{17}O, ^{14}N and ^{2}H nuclei

Nucleus	C_Q (MHz)[a]						η_Q[a]					
	Monomer[b]		Dimer[c]		Lattice[d]		Monomer[b]		Dimer[c]		Lattice[d]	
	Before[e]	After[f]	Before[e]	After[f]	Before[e]	After[f]	Before[e]	After[f]	Before[e]	After[f]	Before[e]	After[f]
^{17}O	10.1 [10.1]	9.90 [9.86]	9.54 [9.48]	9.17 [9.09]	8.81 [8.76]	8.48 [8.45]	0.12 [0.13]	0.16 [0.17]	0.25 [0.26]	0.32 [0.33]	0.42 [0.44]	0.51 [0.52]
^{14}N	3.58 [3.70]	4.27 [4.43]	3.06 [3.18]	3.55 [3.70]	2.53 [2.64]	2.86 [3.01]	0.22 [0.17]	0.08 [0.09]	0.39 [0.33]	0.38 [0.36]	0.65 [0.56]	0.32 [0.25]
$^{2}H1$	547 [532]	266 [255]	551 [538]	230 [220]	522 [507]	236 [226]	0.12 [0.11]	0.17 [0.16]	0.13 [0.13]	0.20 [0.20]	0.11 [0.11]	0.19 [0.18]
$^{2}H2$	653 [636]	262 [250]	671 [655]	263 [251]	630 [613]	220 [211]	0.12 [0.11]	0.19 [0.18]	0.11 [0.10]	0.17 [0.16]	0.11 [0.10]	0.19 [0.18]
^{2}H	377 [369]	202 [194]	378 [370]	205 [196]	368 [360]	181 [176]	0.02 [0.02]	0.02 [0.02]	0.02 [0.02]	0.03 [0.02]	0.02 [0.03]	0.04 [0.04]

[a] The values in brackets are for 6-311+G* basis set and those out of brackets are for 6-311++G** one. The C_Q values of ^{2}H are in kHz.
[b] Crystalline monomer.
[c] Crystalline dimer including the target and molecule No. 3 (see Fig. 1), the values are averaged for two molecules.
[d] The target molecule in lattice (see Fig. 1).
[e] Before H-optimization.
[f] After H-optimization.

Table 3
The CS tensors at the sites of ^{17}O, ^{15}N and ^{1}H nuclei

Nucleus	σ_{iso} (ppm)[a]					
	Monomer[b]		Dimer[c]		Lattice[d]	
	Before[e]	After[f]	Before[e]	After[f]	Before[e]	After[f]
^{17}O	−106 [−102]	−94 [−90]	−62 [−58]	−49 [−46]	−20 [−16]	−4.7 [−1.7]
^{15}N	170 [171]	148 [149]	154 [155]	133 [134]	143 [144]	118 [119]
$^{1}H1$	31 [32]	27 [28]	27 [28]	23 [24]	28 [29]	23 [24]
$^{1}H2$	32 [33]	27 [28]	32 [32]	27 [28]	29 [30]	23 [24]
^{1}H	34 [34]	30 [31]	34 [34]	32 [32]	33 [33]	29 [30]

[a] The values in brackets are for 6-311+G* basis set and those out of brackets are for 6-311++G** one.
[b] Crystalline monomer.
[c] Crystalline dimer including the target and molecule No. 3 (see Fig. 1), the values are averaged for two molecules.
[d] The target molecule in lattice (see Fig. 1).
[e] Before H-optimization.
[f] After H-optimization.

evaluated by the calculated CS tensors at the sites of ^{17}O, ^{15}N and ^{1}H nuclei for three forms of monomer, dimer and the target molecule in lattice of crystalline acetamide.

2. Computational details

Quantum chemical calculations were carried out at the level of density functional theory (DFT) using Gaussian 98 package of program [18]. B3LYP exchange-functional method and 6-311++G** and 6-311+G* standard basis sets were employed in the EFG and CS tensors calculations. The gauge-included atomic orbital (GIAO) approach [19] was used to calculate the CS tensors. Since the considered coordinates of acetamide was obtained from available X-ray study [17] (see Fig. 1), no optimization was needed to perform on the considered structure. However, because the hydrogen positions are not accurately located by X-ray, just these positions in each of the considered monomer and lattice forms of acetamide were allowed relax during the optimization at the theory level of BLYP/6-31G* while other atoms positions were remained frozen during the process (see Table 1).

Quantum chemical calculations yield the EFG and CS tensors eigenvalues in the principal axes system (PAS) [20]. Therefore, relating directly with the experiment, the EFG tensors ($|q_{zz}| > |q_{yy}| > |q_{xx}|$) were converted to the experimentally measurable parameters, quadrupole coupling constant and asymmetry parameter (see Eqs. (1) and (2)). C_Q refers to the interaction energy of electric quadrupole moment (eQ) of the quadrupole nucleus with the EFG tensor and η_Q refers to the deviation of electronic distribution around the quadrupole nucleus from the cylindrical symmetry. In Eq. (1), the standard values of $Q(^{17}O) = 25.58$ mb, $Q(^{14}N) = 20.44$ mb and $Q(^{2}H) = 2.56$ mb reported by Pyykkö [21] are used. The evaluated C_Q and η_Q at the sites of ^{17}O, ^{14}N and ^{2}H nuclei in the forms of monomer, dimer and the target molecule in lattice of acetamide before and after H-optimization are presented in Table 2.

$$C_Q(\mathrm{MHz}) = e^2 Q q_{zz}\ \mathrm{h}^{-1} \quad (1)$$

$$\eta_Q = \left| \frac{q_{xx} - q_{yy}}{q_{zz}} \right| \quad (2)$$

The calculated CS tensor in the PAS ($\sigma_{33} > \sigma_{22} > \sigma_{11}$) were converted to the isotropic chemical shielding by Eq. (3) and the σ_{iso} at the sites of ^{17}O, ^{15}N and ^{1}H nuclei in the forms of monomer, dimer and the target molecule in lattice of acetamide before and after H-optimization are summarized in Table 3.

$$\sigma_{iso}(\mathrm{ppm}) = \frac{\sigma_{11} + \sigma_{22} + \sigma_{33}}{3} \quad (3)$$

3. Results and discussion

The EFG tensors at the sites of ^{17}O, ^{14}N and ^{2}H nuclei (see Table 2) and the CS tensors at the sites of ^{17}O, ^{15}N and ^{1}H nuclei (see Table 3) were calculated to study the HB interactions properties of O=C–NH group in acetamide (see Fig. 1). To this aim, the crystalline structure of acetamide was obtained from earlier X-ray study [17] and considered in the NMR calculations. It is noted that to investigate the HB properties of O=C–NH group, the NMR calculations were performed on monomer, dimer and lattice forms of crystalline acetamide. The most HB interacting molecules through N–H···O and C–H···O HB types with the target one were considered in a six-molecule lattice form of acetamide by the X-ray coordinates transforming (see Table 1 and Fig. 1). However, the representative dimer model consists of just two molecules which are in the most HB contributions together. Furthermore, since H positions are not accurately located by X-ray, just these positions were optimized at the theory level of BLYP/6-31G* (see Table 1) and NMR calculations were performed on each of monomer, dimer and lattice forms of acetamide before and after H-optimization to show the importance of this process in considering X-ray structures in the calculations. It is noted that since the two molecules of dimer model are in the same condition of contributing to HB, their average calculated NMR parameters at the sites of each nucleus are reported. The following text will discuss the calculated EFG and CS tensors at the sites of various nuclei in monomer, dimer and the target molecule in lattice of

crystalline acetamide, respectively, which the results of 6-311++G** employed basis set are referred to.

3.1. Electric field gradient tensors

In this section, the calculated EFG tensors at the sites of ^{17}O, ^{14}N and ^{2}H nuclei in monomer, dimer and the target molecule in lattice forms of acetamide before and after H-optimization are discussed (see Table 1 and Fig. 1). As mentioned earlier, to directly relate with the experiment, the calculated EFG tensors were converted to the experimentally measurable parameters, quadrupole coupling constant and asymmetry parameter using Eqs. (1) and (2) and the evaluated values of C_Q and η_Q at the sites of ^{17}O, ^{14}N and ^{2}H nuclei are presented in Table 2.

The oxygen of peptide group (O=C–NH) in the target molecule of acetamide contributes to three HB interactions through two types of N–H···O and C–H···O ones with three neighboring molecules in the lattice (see Table 1 and Fig. 1). Therefore, the C_Q and η_Q parameters at the site of ^{17}O are significantly influenced by HB from the monomer to the target molecule in lattice (see Table 2). However, from monomer to dimer models, less influence is observed revealing the importance of considered models in the calculations to interpret HB properties. As mentioned earlier, the H positions were just optimized in the considered crystalline structure of acetamide in all forms of monomer, dimer and lattice ones and the difference between the geometrical properties before and after this process are exhibited in Table 1. Due to the relationship between the geometrical properties of structures and NMR parameters [22], the calculated NMR parameters in monomer and dimer forms of acetamide before and after H-optimization are significantly different. In lattice form, since the intermolecular geometrical properties of HB interactions are changed by optimization of H positions, different NMR parameters are also calculated in lattice forms of acetamide before and after H-optimization.

In the after H-optimization case, $C_Q(^{17}O)$ reduces 1.42 MHz and $\eta_Q(^{17}O)$ increases 0.35 from monomer to the target molecule in lattice. The significant changes of C_Q and η_Q values reveal that the EFG tensors at the site of ^{17}O are significantly influenced by three HB interactions with molecules No. 3, No. 4 and No. 5 which among them the target molecule contributes to classical HB type of N–H···O with molecules No. 3 and No. 4, however, it interacts with molecule No. 4 through the non-classical HB type of C–H···O one. From the X-ray study [17], the weak C–H···O type of HB interaction is very important in the connections of neighboring columns of acetamide, therefore, its characterization is an interesting task. To more characterize the properties of C–H···O type of HB contribution of peptide group in acetamide, the changes of EFG tensors at the site of that ^{2}H chemically bonded to C2 are used as evidence. This H contributes to C–H···O type of HB interaction with molecule No. 6 and because of this interaction, $C_Q(^{2}H)$ reduces 21 kHz from monomer to the target molecule in lattice which is such a significant change of EFG tensors at the sites of ^{2}H nuclei and reveals the importance of C–H···O type of HB interaction of the peptide group in acetamide. –NH2 group plays major roles in biological systems especially in contributing to strong HB interactions. Nitrogen of peptide group in the target molecule of acetamide contributes to N–H···O type of HB interactions with molecule No. 2 and No. 3 in lattice (see Table 1 and Fig. 1). In the after H-optimization case, $C_Q(^{14}N)$ reduces 1.41 MHz and $\eta_Q(^{14}N)$ increases 0.24 from monomer to the target molecule in lattice of acetamide which reveals the importance of –NH2 group in HB interaction properties of peptide group in acetamide. Although the hydrogen nucleus has a very poor electronic environment, however, the EFG tensors at the sites of $^{2}H1$ and $^{2}H2$ nuclei also undergo significant changes in the presence of N–H···O type of HB interactions which shows the sensitivity of the EFG tensors to the HB interactions effects. The C_Q values of $^{2}H1$ and $^{2}H2$ reduce 30 and 42 kHz, respectively, from monomer to the target molecule in lattice. From Table 1, contribution of H2 to N–H···O type of HB interaction with molecule No. 2 is in a better intermolecular geometrical properties rather than that of H1 with molecule No. 3, therefore, $C_Q(^{2}H2)$ undergoes more reduction regarding to $C_Q(^{2}H1)$ because of HB interaction in lattice of acetamide. To best of our knowledge, to this point, there is no experimental NMR data for acetamide. However, comparison with the calculated C_Q parameters of *N*-methylacetamide (NMA) reported by Ludwig et al. [8] reveals that acetamide contributes to more HB interactions rather than NMA and, therefore, the C_Q parameters undergo more changes by including HB interactions in acetamide.

3.2. Chemical shielding tensors

The calculated CS tensors at the sites of ^{17}O, ^{15}N and ^{1}H nuclei in all of monomer, dimer and lattice forms of crystalline acetamide (see Table 1 and Fig. 1) in order to characterize the peptide group (O=C–NH) HB properties are discussed here. The evaluated values of isotropic chemical shielding from the calculated CS tensors by Eq. (3) are exhibited in Table 3. As mentioned above, in the previous section, it was shown that the EFG tensors at the sites of peptide group nuclei are significantly influenced by HB interactions in which from monomer to the target molecule in lattice it is more significant rather than to dimer model. Since both EFG tensors and CS tensors are originated by electronic environment at the sites of nuclei, it is expected that they undergo parallel changes in the presence of HB interactions. Previous works [15,16] also showed that the calculation of both tensors is an advantage in the interpretation of HB properties in the considered systems of study.

The evaluated σ_{iso} at the site of ^{17}O reveals that because of contributing to three HB interactions with three neighboring molecules, the $\sigma_{iso}(^{17}O)$ of the peptide group shifts about 90 ppm from monomer to the target molecule in lattice of acetamide in the H-optimized case. As mentioned earlier, this trend reveals that the EFG and CS tensors undergo parallel changes due to HB interactions effects, however, the magnitude of change is not equal sometimes. $\sigma_{iso}(^{14}N)$ also shifts 30 ppm from monomer to the target molecule in lattice. Because of the low electronic density of hydrogen nucleus, $\sigma_{iso}(^{1}H)$ undergoes just about 4 ppm at the sites of $^{1}H1$ and $^{1}H2$ from monomer to

the target molecule in lattice. Comparisons with the EFG tensors, the CS tensors results reveal that in the same condition of HB interactions, EFG tensors are more sensitive regarding to the CS tensors, but both of them are very important and helpful parameters in the interpretation of HB interactions properties and also prove each other. $\sigma_{iso}(^1H)$ at the site of H nucleus which is contributed to C–H···O type of HB interaction undergoes a 1 ppm shift from monomer to the target molecule in lattice of crystalline acetamide. Parallel with the C_Q results of Ludwig et al. [8] discussed above, the isotropic chemical shieldings also undergo more changes by including HB interactions in acetamide rather than those of NMA.

4. Conclusion

We performed a DFT study to investigate the HB interactions properties of the peptide group (O=C–NH) in crystalline acetamide. To this aim, the EFG tensors at the sites of ^{17}O, ^{14}N and ^2H nuclei and the CS tensors at the sites of ^{17}O, ^{15}N and ^1H nuclei in monomer and lattice forms of crystalline acetamide were calculated and converted to the measurable parameters of C_Q, η_Q and σ_{iso}. From the evaluated NMR parameters, some trends are obtained. First, since the NMR parameters at the sites of peptide group nuclei are significantly changed from monomer to the target molecule in lattice of crystalline acetamide, the peptide group contributes to major HB interactions with neighbor molecules. Second, N–H···O type of HB interaction plays the major role in lattice of crystalline acetamide. Third, although the non-classical C–H···O type of HB interaction is not strong, however, its influence especially on the EFG tensors at the site of ^2H nuclei cannot be neglected. Fourth, and finally, since X-ray cannot accurately locate hydrogen positions in crystals, their optimization is an essential task in considering the X-ray crystals in the calculations.

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