

Hydrogen Bonds of Peptide Group in Four Acetamide Derivatives: DFT Study of Oxygen and Nitrogen NQR and NMR Parameters

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Z.S. respectfully dedicates this work to the memory of her husband, Dr. Yahya Emami.

A computational study was conducted to examine hydrogen bond (HB) properties of peptide group in four derivatives of acetamide by density functional theory (DFT) calculations of nuclear quadrupole resonance (NQR) and nuclear magnetic resonance (NMR) parameters at the sites of oxygen and nitrogen nuclei of peptide groups. The available crystalline structures of four derivatives; 2,2,2-trifluoro-N-(2-hydroxy-5-nitrophenyl)acetamide, N-(2-acetylphenyl)acetamide, 2-chloro-N-(4-nitrophenyl)acetamide, and N-(4-fluorophenyl)acetamide were obtained from literature. Following the influence of HB interactions, calculations were done on non-hydrogen bonded (single) and hydrogen bonded (cluster) models of derivatives. The results revealed different behaviors of peptide group in contributing to HB interactions in different derivative structures. HB interactions are the strongest in 2-chloro-N-(4-nitrophenyl)acetamide. However, the strengths of HB interactions in all of the four derivatives are still less than that of acetamide. The calculations are done at the level of B3LYP method and 6-311++G** standard basis set using GAUSSIAN 98 package of program.

Keywords: Acetamide, Peptide, Hydrogen bond, Electric field gradient, Chemical shielding

INTRODUCTION

Numerous studies have been devoted to investigate the hydrogen bond (HB) features in the natural phenomena, especially in biological systems. Indeed, HB plays an essential role in accurate structural determination of polypeptides in proteins [1]. Since the structures of macromolecular proteins in living systems are very complex, studying the simplest models having the major characteristic of proteins is an advantage in the investigation of HB properties in these structures. Acetamide (Fig. 1), which has a single peptide

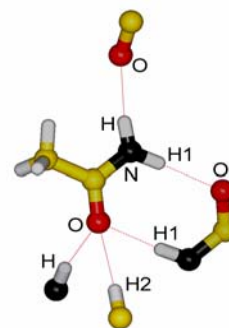


Fig. 1. Cluster of acetamide. Dash lines show HB interactions. For the sake of simplicity, just the interacting parts of four neighbor molecules are shown (Table 1), see Ref. [20].

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group (O=C-NH), is the simplest model system of peptide linkage in proteins and polypeptides. Acetamide and some of its derivatives are capable of contributing to N-H \cdots O=C and C-H \cdots O=C types of HB interactions. Numerous studies using various techniques have focused on the characterization of properties of these HB interactions in α -helix and β -sheet stabilizations [2-14].

A variety of theoretical and experimental methods are employed to obtain information about the properties of HB interactions. However, nuclear quadrupole resonance (NQR) and nuclear magnetic resonance (NMR) spectroscopies are among the most efficient techniques for the purpose [15,16]. Measuring the electric field gradient (EFG) and chemical shielding (CS) tensors provides important information about the electronic sites of those quadrupole nuclei, *e.g.*, ^{17}O and ^{14}N , and magnetic nuclei, *e.g.*, ^{17}O and ^{15}N , which contribute to HB interactions [17-19].

In a recent work [20], we studied the HB properties of peptide group in crystalline structure of acetamide. However, due to the importance of peptide group in polypeptides and proteins, the HB properties of this group in four crystalline derivatives of acetamide are further studied in the present work. The crystalline structures of acetamide derivatives are 2,2,2-trifluoro-N-(2-hydroxy-5-nitrophenyl)acetamide (Fig. 2) [21], N-(2-acetylphenyl)acetamide (Fig. 3) [22], 2-chloro-N-(4-nitrophenyl)acetamide (Fig. 4) [23], and N-(4-fluorophenyl)acetamide (Fig. 5) [24]. NQR and NMR parameters are calculated at the sites of oxygen and nitrogen nuclei of peptide group to examine the HB properties of O=C-NH in the above-mentioned derivatives of acetamide (Tables 2 and 3).

COMPUTATIONAL DETAILS

The quantum chemical calculations in this study are done at the level of density functional theory (DFT) using GAUSSIAN 98 package of program [25]. The crystalline structures of acetamide derivatives are obtained from literature; 2,2,2-trifluoro-N-(2-hydroxy-5-nitrophenyl)acetamide (Fig. 2) [21], N-(2-acetylphenyl)acetamide (Fig. 3) [22], 2-chloro-N-(4-nitrophenyl)acetamide (Fig. 4) [23], and N-(4-fluorophenyl)acetamide (Fig. 5) [24]. The contribution of peptide group to HB interactions is also considered in calculations by including the most possible interacting

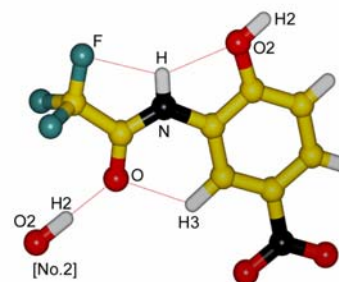


Fig. 2. Cluster of 2,2,2-Trifluoro-N-(2-hydroxy-5-nitrophenyl)acetamide. Dash lines show HB interactions. For the sake of simplicity, just the interacting parts of one neighbor molecule are shown. Complete structure is considered in the calculations (Table 1).

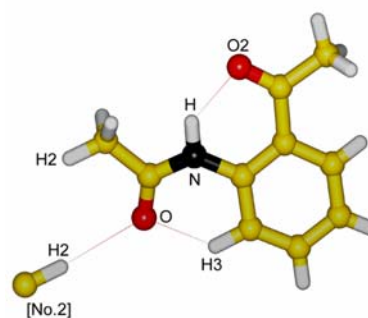


Fig. 3. Cluster of N-(2-acetylphenyl)acetamide. Dash lines show HB interactions. For the sake of simplicity, just the interacting parts of one neighbor molecule are shown. Complete structure is considered in the calculations (Table 1).

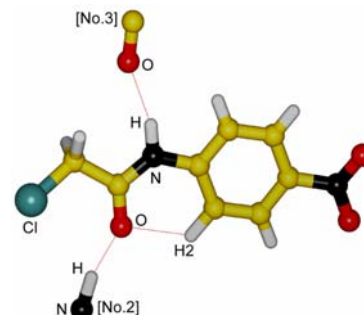


Fig. 4. Cluster of 2-Chloro-N-(4-nitrophenyl)acetamide. Dash lines show HB interactions. For the sake of simplicity, just the interacting parts of two neighbor molecules are shown. Complete structure is considered in the calculations (Table 1).

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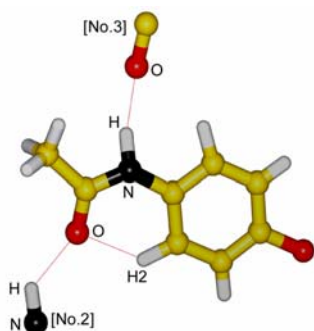


Fig. 5. Cluster of N-(4-fluoro phenyl)acetamide. Dash lines show HB interactions. For the sake of simplicity, just the interacting parts of two neighbor molecules are shown. Complete structure is considered in the calculations (Table 1).

neighbor molecules with the target molecule by transformations of the available x-ray coordinates (Table 1 and Figs. 2-5). Additionally, to compare the influence of HB interactions on the electronic sites of oxygen and nitrogen

nuclei of peptide group, the calculations are done for both of hydrogen bonded (cluster) and non-hydrogen bonded (single) structures (Tables 2 and 3).

There are two molecules in cluster models of the first and the second derivatives. Similarly, there are three molecules in cluster models of the third and the fourth derivatives. Considering the real crystalline structures in calculations helps yield more reliable results as well as save time of calculations. However, the positions of hydrogen atoms due to low electron density are not accurately located by x-ray diffraction. Therefore, following the earlier work of Ida *et al.* [26], only the hydrogen positions of peptide group in the single and cluster structures are separately optimized at the level of B3LYP method and 6-311++G** standard basis set while the other atoms positions are kept frozen during the process.

The EFG tensors at the sites of ^{17}O and ^{14}N nuclei of peptide group are calculated at the level of B3LYP method and 6-311++G** standard basis set. In an earlier study, we indicated that the employed method and basis set yield reliable results without basis set superposition error (BSSE) [19]. The

Table 1. The Geometrical Properties of Hydrogen Bonds^a

Acetamide derivative	Bond lengths (Å)	Bond angles (°)
2,2,2-Trifluoro-N-(2-hydroxy-5-nitrophenyl)acetamide	$r_{\text{H}\cdots\text{O}2} = 2.10$	$\angle_{\text{N-H}\cdots\text{O}2} = 106$
	$r_{\text{H}\cdots\text{F}} = 2.20$	$\angle_{\text{N-H}\cdots\text{F}2} = 103$
	$r_{\text{H}2\cdots\text{O}} = 1.70$	$\angle_{\text{C=O}\cdots\text{H}2} = 133$
	$r_{\text{H}3\cdots\text{O}} = 2.19$	$\angle_{\text{C=O}\cdots\text{H}3} = 105$
N-(2-Acetyl phenyl)acetamide	$r_{\text{H}\cdots\text{O}2} = 1.89$	$\angle_{\text{N-H}\cdots\text{O}2} = 143$
	$r_{\text{H}2\cdots\text{O}} = 2.69$	$\angle_{\text{C=O}\cdots\text{H}2} = 118$
	$r_{\text{H}3\cdots\text{O}} = 2.31$	$\angle_{\text{C=O}\cdots\text{H}3} = 99$
2-Chloro-N-(4-nitrophenyl)acetamide	$r_{\text{H}\cdots\text{O}} = 1.88$	$\angle_{\text{N-H}\cdots\text{O}} = 156$
	$r_{\text{H}2\cdots\text{O}} = 2.20$	$\angle_{\text{C=O}\cdots\text{H}2} = 104$
N-(4-Fluoro phenyl)acetamide	$r_{\text{H}\cdots\text{O}} = 1.84$	$\angle_{\text{N-H}\cdots\text{O}} = 168$
	$r_{\text{H}2\cdots\text{O}} = 2.28$	$\angle_{\text{C=O}\cdots\text{H}2} = 106$
Acetamide ^b	$r_{\text{N}\cdots\text{O}} = 2.87$	$\angle_{\text{N-H}\cdots\text{O}} = 168.3$
	$r_{\text{H}\cdots\text{O}} = 1.86$	$\angle_{\text{N-H}\cdots\text{O}} = 162.6$
	$r_{\text{N}\cdots\text{O}} = 2.93$	$\angle_{\text{O}\cdots\text{H}-\text{N}} = 169.4$
	$r_{\text{H}1\cdots\text{O}} = 1.94$	$\angle_{\text{O}\cdots\text{H}-\text{C}} = 176.4$
	$r_{\text{H}\cdots\text{O}} = 2.37$	$\angle_{\text{O}\cdots\text{H}-\text{N}} = 163.8$

^aData are from Refs. [21-24] but the H positions are optimized. See Figs. 2-5. ^bData are from Ref. [20], see Fig. 1.

Table 2. The Oxygen NQR and NMR Parameters^a

Acetamide derivative	$C_Q(^{17}\text{O})$ (MHz)		$\eta_Q(^{17}\text{O})$		$\sigma_{iso}(^{17}\text{O})$ (ppm)	
	Single ^b	Cluster ^c	Single ^b	Cluster ^c	Single ^b	Cluster ^c
2,2,2-Trifluoro-N-(2-hydroxy-5-nitrophenyl)acetamide	10.2	9.26	0.06	0.17	-85.2	-28.7
N-(2-Acetyl phenyl)acetamide	10.5	10.4	0.07	0.08	-122	-120
2-Chloro-N-(4-nitrophenyl)acetamide	10.5	9.73	0.07	0.19	-123	-72.2
N-(4-Fluoro phenyl)acetamide	10.2	9.63	0.02	0.18	-109	-100
Acetamide ^d	9.90	8.48	0.16	0.51	-94	-4.7

^aThe values are for peptide group (Figs. 1-5). ^bThe H positions are optimized in crystalline monomer. ^cThe H positions are optimized in crystalline cluster. ^dData are from Ref. [20].

Table 3. The Nitrogen NQR and NMR Parameters^a

Acetamide derivative	$C_Q(^{14}\text{N})$ (MHz)		$\eta_Q(^{14}\text{N})$		$\sigma_{iso}(^{15}\text{N})$ (ppm)	
	Single ^b	Cluster ^c	Single ^b	Cluster ^c	Single ^b	Cluster ^c
2,2,2-Trifluoro-N-(2-hydroxy-5-nitrophenyl)acetamide	3.56	3.30	0.32	0.34	127	123
N-(2-acetyl phenyl)acetamide	3.29	3.13	0.58	0.85	109	120
2-Chloro-N-(4-nitrophenyl)acetamide	4.13	3.45	0.12	0.39	112	103
N-(4-Fluoro phenyl) acetamide	4.07	3.31	0.15	0.42	107	100
Acetamide ^d	4.27	2.86	0.08	0.32	148	118

^aThe values are for peptide group (Figs. 1-5). ^bThe H positions are optimized in crystalline monomer. ^cThe H positions are optimized in crystalline cluster. ^dData are from Ref. [20].

calculated EFG tensors are directly converted to the experimentally measurable NQR parameters, quadrupole coupling constant (C_Q) and asymmetry parameter (η_Q), using Eqs. (1) and (2). Note that the standard values of Q reported by Pyykkö²⁷ are employed in Eq. (1); $Q(^{17}\text{O}) = 25.58$ mb, $Q(^{14}\text{N}) = 20.44$ mb. NQR deals with the nuclei with nuclear spin angular momentum (I) greater than one-half *e.g.*, ^{17}O and ^{14}N . The electric quadrupole moment (eQ) of these nuclei interacts with the EFG tensors where the interaction energy is defined by C_Q . The deviations of the EFG tensors from cylindrical symmetry at the sites of quadrupole nuclei are

defined by η_Q .

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

$$\eta_Q = |(q_{xx} - q_{yy})/q_{zz}|; (|q_{xx}| < |q_{yy}| < |q_{zz}|). \quad (2)$$

The CS tensors at the sites of ^{17}O and ^{15}N nuclei of peptide group are calculated at the level of B3LYP method and 6-311++G** standard basis set based on the gauge independent atomic orbital (GIAO) approach [28]. The calculated CS tensors are converted to the experimentally measurable NMR

parameter, isotropic chemical shielding (σ_{iso}), using Eq. (3).

$$\sigma_{iso} \text{ (ppm)} = (\sigma_{11} + \sigma_{22} + \sigma_{33})/3 ; (\sigma_{11} < \sigma_{22} < \sigma_{33}) \quad (3)$$

RESULTS AND DISCUSSIONS

In this work, the HB properties of peptide group (O=C-NH) are studied by calculations of oxygen and nitrogen NQR and NMR parameters in four crystalline structures of acetamide derivatives. The evaluated quadrupole coupling constant (C_Q) and asymmetry parameter (η_Q) at the sites of ^{17}O and ^{14}N nuclei and the isotropic chemical shielding (σ_{iso}) at the sites of ^{17}O and ^{15}N nuclei of peptide group in both non-hydrogen bonded (single) and hydrogen bonded (cluster) systems are exhibited in Tables 2 and 3. The available NQR and NMR data calculated for crystalline acetamide are also included in the tables [20]. In the following sections, we discuss the HB properties of peptide group in each of the acetamide derivatives separately.

2,2,2-Trifluoro-N-(2-hydroxy-5-nitrophenyl)acetamide

The available crystalline structure of 2,2,2-Trifluoro-N-(2-hydroxy-5-nitrophenyl)acetamide [21] shows that the peptide group in this acetamide derivative contributes to one neighbor molecule through intermolecular C=O \cdots H-O type of HB interactions (Table 1 and Fig. 2). In addition, the peptide group also contributes to intramolecular C=O \cdots H-C, N-H \cdots O-C, and N-H \cdots F-C types of HB interactions. Hence, the calculated NQR and NMR parameters at the sites of oxygen and nitrogen nuclei of peptide group are changed from single to cluster model (Tables 2 and 3). Although the intramolecular HB interaction also exists in single model, however, contributing to intermolecular HB interaction with molecule number two causes C_Q , η_Q , and σ_{iso} undergo changes.

Comparing the results with recent study of acetamide [20] indicates that the NQR and NMR parameters at the sites of oxygen and nitrogen nuclei of this derivative are less influenced by HB interactions than by those of acetamide. However, the changes are also significant in 2,2,2-Trifluoro-N-(2-hydroxy-5-nitrophenyl)acetamide. Due to HB interactions, $C_Q(^{17}\text{O})$ decreases 0.94 MHz and $\eta_Q(^{17}\text{O})$

increases 0.11 from single to cluster model. $\sigma_{iso}(^{17}\text{O})$ also goes 56.5 ppm to upper fields. Since N-H does not contribute to intermolecular HB interactions because of some intramolecular HB interactions and presence in cluster, $C_Q(^{14}\text{N})$ decreases 0.26 MHz and $\eta_Q(^{14}\text{N})$ increases 0.02 from single to cluster model both of which are less significant than those of oxygen nuclei parameters. The change of $\sigma_{iso}(^{15}\text{N})$ is a negligible value of 4 ppm. Compared with the HB interactions of acetamide, the contribution of 2,2,2-Trifluoro-N-(2-hydroxy-5-nitrophenyl)acetamide to the HB interactions lessens with the oxygen nuclei playing the major role in intermolecular interactions of this acetamide derivative crystal cluster.

N-(2-Acetylphenyl)acetamide

The reported crystalline structure of N-(2-acetylphenyl)acetamide [22] shows that the peptide group of target molecule contributes to intermolecular HB interaction with only one neighboring molecule through C=O \cdots H-C type (Table 1 and Fig. 3). There are also two intramolecular HB interactions of C=O \cdots H-C and N-H \cdots O=C types. Oxygen just contributes to two C=O \cdots H-C HB interactions which are classified as weak non-classical types of HB interactions. Therefore, the NQR and NMR parameters at the site of this nucleus undergo slight changes. From single to cluster model, $C_Q(^{17}\text{O})$ is reduced to 0.1 MHz, $\eta_Q(^{17}\text{O})$ increases 0.01, and $\sigma_{iso}(^{17}\text{O})$ goes just 2 ppm to upper fields due to HB interactions. Being in cluster causes more changes in the NQR and NMR parameters of nitrogen than those of oxygen, $C_Q(^{14}\text{N})$ is reduced to 0.16 MHz, $\eta_Q(^{14}\text{N})$ increases 0.27, and $\sigma_{iso}(^{15}\text{N})$ goes 11 ppm to lower fields from single to cluster model. This trend reveals the major contribution of nitrogen to HB interactions rather than that of oxygen in crystal cluster of N-(2-acetylphenyl)acetamide. Compared with acetamide, it also reveals that the strength of HB interactions in N-(2-acetylphenyl)acetamide still lessens.

2-Chloro-N-(4-nitrophenyl)acetamide

2-Chloro-N-(4-nitrophenyl)acetamide contributes to intermolecular N-H \cdots O=C type of HB interaction with two neighboring molecules in reported crystalline structure [23] (Table 1 and Fig. 4). Oxygen of peptide group also contributes to intramolecular C=O \cdots H-C type of HB interaction. Due to

HB interactions, the NQR and NMR parameters at the sites of oxygen and nitrogen nuclei of this acetamide derivative undergo changes; however, the magnitude of change is still less than that of acetamide. $C_Q(^{17}\text{O})$ is reduced 0.78 MHz, $\eta_Q(^{17}\text{O})$ increases 0.12, and $\sigma_{iso}(^{17}\text{O})$ goes 50.8 ppm to upper fields due to HB interactions. In addition, $C_Q(^{14}\text{N})$ is reduced to 0.68 MHz, $\eta_Q(^{14}\text{N})$ increases 0.27, and $\sigma_{iso}(^{15}\text{N})$ goes 9 ppm to upper fields due to HB interactions. Although the changes in the NQR and NMR parameters at the sites of oxygen and nitrogen nuclei of this derivative due to HB interactions are more than those of two previous derivatives, however, the magnitude of changes are still less than those of acetamide. But a significant trend about 2-chloro-N-(4-nitrophenyl)acetamide is that both oxygen and nitrogen nuclei have the major contributions to HB interactions in this crystal cluster.

N-(4-Fluorophenyl)acetamide

N-(4-fluorophenyl)acetamide contributes to intermolecular N-H \cdots O=C type of HB interaction with two neighboring molecules in reported crystalline structure [24] (Table 1 and Fig. 5). Oxygen of peptide group also contributes to intramolecular C=O \cdots H-C type of HB interaction. From single to cluster model, the NQR and NMR parameters at the sites of oxygen and nitrogen nuclei of this acetamide derivative undergo changes due to HB interactions. $C_Q(^{17}\text{O})$ is reduced to 0.57 MHz, $\eta_Q(^{17}\text{O})$ increases 0.16, and $\sigma_{iso}(^{17}\text{O})$ goes 9 ppm to upper fields due to HB interactions. Additionally, $C_Q(^{14}\text{N})$ is reduced to 0.76 MHz, $\eta_Q(^{14}\text{N})$ increases 0.27, and $\sigma_{iso}(^{15}\text{N})$ goes 7 ppm to upper fields due to HB interactions. Parallel to 2-chloro-N-(4-nitrophenyl)acetamide, the changes in the NQR and NMR parameters at the sites of oxygen and nitrogen nuclei of this derivative due to HB interactions are more than those of the two other derivatives and also significant. In this derivative, both oxygen and nitrogen nuclei have the major contributions to HB interactions in crystal cluster. However, compared with acetamide, the strength of HB interactions is still less here.

CONCLUSIONS

We carried out a computational study on four derivatives of acetamide to examine the properties of HB interaction of peptide group by DFT calculations of NQR and NMR

parameters at the sites of oxygen and nitrogen nuclei. The results reveal that due to HB interactions the parameters change from single to cluster models. Moreover, the strength of HB interactions is different in various derivatives though weaker than that of acetamide. The NQR and NMR parameters at the sites of oxygen and nitrogen nuclei are significantly influenced in 2-chloro-N-(4-nitrophenyl)acetamide where both oxygen and nitrogen nuclei contribute to HB interactions in cluster. In cluster of N-(4-fluorophenyl)acetamide, oxygen and nitrogen also contribute to HB interactions, however, the strength is slightly weaker than 2-chloro-N-(4-nitrophenyl)acetamide. In cluster of N-(2-acetylphenyl)acetamide nitrogen plays the major role while in cluster of 2,2,2-Trifluoro-N-(2-hydroxy-5-nitrophenyl)acetamide the oxygen plays the major role of HB interactions. Therefore, the changes in NQR and NMR parameters are significantly less than the other two derivatives.

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