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A density functional study of ^{17}O, ^{14}N and ^{2}H electric field gradient tensors in the real crystalline structure of α-glycine

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Abstract

A density functional theory (DFT) study was carried out to calculate ^{17}O, ^{14}N and ^{2}H electric field gradient (EFG) tensors in accurate neutron diffraction structures of α-glycine at 288 and 427 K. B3LYP is the used method and 6-311+G* and 6-311++G** are the basis sets in the calculations of EFG tensors at the sites of ^{17}O, ^{14}N and ^{2}H nuclei in the monomer and the octameric cluster of α-glycine at two temperatures. Quadrupole coupling constants and asymmetry parameters are the converted parameters of calculated EFG tensors to experimentally measurable ones. The calculated results of monomer and the target molecule in octameric cluster reveal that hydrogen-bonding interactions play an important role in the crystalline structure of α-glycine where the results of the target molecule in octameric cluster are in good agreement with the experiments.

Keywords: DFT; EFG; α-Glycine; N–H...O hydrogen bond; C–H...O hydrogen bond

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1. Introduction

The electric field gradient (EFG) tensors arisen at the sites of quadrupole nuclei are important physical parameters to investigate the structural properties of molecules [1,2]. Those nuclei with spin angular momentum greater than one-half ($I > 1/2$) are quadrupole and have electric quadrupole moment, eQ, which can interact with the EFG tensors [3]. The strength of this interaction depends on the magnitude of eQ and the EFG eigenvalues. Since the EFG tensors are very sensitive to the electrostatic environment of nuclei, intermolecular interactions e.g. hydrogen bonding (HB) interactions, have significant influence on the EFG tensors. The quantum calculations yield the EFG tensors in the principal axis system, PAS, where can be converted to the experimentally measurable parameters quadrupole coupling constants, C_Q, and asymmetry parameters, η_Q.

Glycine, the simplest form of the 20 standard amino acids, is one of the principal components of proteins which participate in several important reactions such as biosynthesis of heme, serine and glutathione. Depending on pH, glycine can have different forms of cationic, anionic and zwitterionic where zwitterionic has three polymorphic forms, α, β and γ in solid-phase [4].

Previously, it has been shown that chemical shifts (CS) and EFG tensors in amino acids are sensitive to the lattice effects such as HB interactions [5–8]. Therefore, to reproduce accurate EFG tensors, intermolecular HB interactions must be considered in the calculations as much closer to experiment as possible. Earlier, Yates and co-workers [9] studied the influence of HB interaction on the ^{17}O EFG tensors in three polymorphs of Glutamic amino acid. Strohmeier and co-workers [10] also considered HB interaction effects in the calculation of NMR parameters for some amino acids. Ando and co-workers [11–18] performed numerous experimental and theoretical studies on the amino acids, peptides and polypeptides to demonstrate the relationship between ^{1}H, ^{13}C, ^{15}N and ^{17}O NMR tensors and hydrogen-bond length.

Present work studies the ^{17}O, ^{14}N and ^{2}H EFG tensors in the α-glycine structure via density functional theory (DFT) where the crystalline coordinates of α-glycine at 288 K and 427 K

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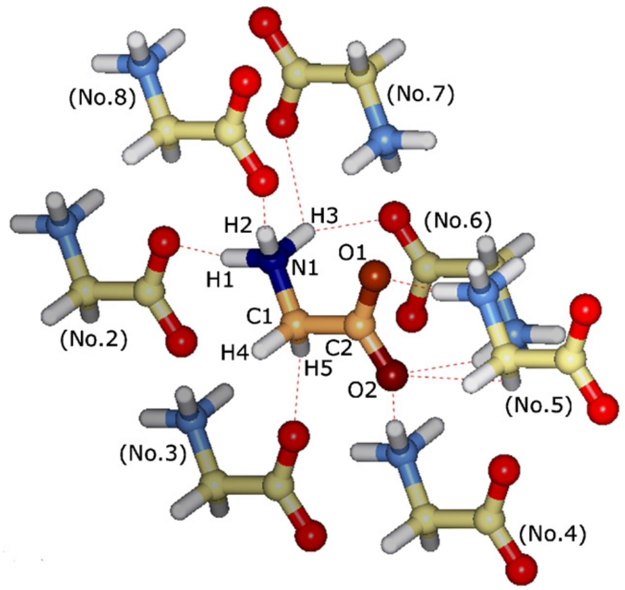

Fig. 1. Structure of α-glycine octamer in solid phase. The target molecule: (*x*, *y*, *z*); No.2: (*x*, *y*, *z*−1); No.3: (*x*−1, *y*, *z*−1) No.4: (*x*−1, *y*, *z*); No.5: (*x*, *y*, *z*+1); No.6: (−*x*, −*y*, −*z*); No.7: (−*x*+1, −*y*, −*z*); No.8: (*x*+1,*y*,*z*).

were obtained from recent neutron diffraction study [4]. Since α-glycine contributes to hydrogen-bonding interactions in the solid-phase, N–H...O and C–H...O HB types, as shown in the recent studies [19–22], those most interacting molecules with the target one were considered in an octameric cluster in the EFG calculations, see Fig. 1. To systematically investigate the HB effects on the EFG tensors, the calculations were also performed on the monomer glycine. The converted ^{17}O, ^{14}N and ^{2}H calculated EFG tensors eigenvalues to those experimentally measurable parameters, quadrupole coupling constants and asymmetry parameter are summarized in Tables 2 and 3.

2. Computational details

All the quantum chemical calculations of ^{17}O, ^{14}N and ^{2}H EFG tensors in the structure of α-glycine were performed at the level of density functional theory (DFT) [23] via Gaussian 98 package [24]. The employed DFT method is B3LYP and the basis sets are 6-311++G** and 6-311+G* which yield reliable calculated EFG tensors [25,26]. It is noteworthy that DFT calculations are performed at 0 K, however, two octameric clusters of α-glycine ($^{+}NH_3CH_2COO^{-}$) were created using neutron diffraction study coordinates at 288 K and 427 K [4] and considered in the calculations, see Fig. 1 and Table 1 for details. Since the positions of hydrogen atoms are determined accurately by neutron diffraction, no geometry optimization was needed in this work. The calculations were also performed on monomer α-glycine to systematically investigate the HB effects on the ^{17}O, ^{14}N and ^{2}H EFG tensors in the α-glycine crystalline structure.

The calculated EFG tensors eigenvalues ($|q_{zz}|>|q_{yy}|>|q_{xx}|$) in the principal axis system (PAS) can be converted to the experimentally measurable parameters using Eqs. (1) and (2). Quadrupole coupling constant, C_Q, is the interaction energy of electric quadrupole moment, eQ, with the EFG tensors at the site of quadrupole nucleus. Another useful parameter is asymmetry parameter, η_Q, which measures the deviation of EFG tensors form axial symmetry.

$$C_Q(\mathrm{MHz}) = e^2Qq_{zz}/h \tag{1}$$

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

In Eq. (1), the standard values of Q reported by Pyykkö [27] are employed: $Q(^{17}O)=25.58$ mb, $Q(^{14}N)=20.56$ mb and $Q(^{2}H)=2.86$ mb. Tables 2 and 3 present the calculated ^{17}O, ^{14}N and ^{2}H C_Q and η_Q parameters for crystalline monomer and the target molecule in crystalline octamer of α-glycine at 288 k and 427 K.

3. Results and discussion

This work calculates ^{17}O, ^{14}N and ^{2}H EFG tensors in α-glycine structure. To consider HB effects in the calculations, octameric clusters of α-glycine were created using neutron diffraction coordinates at 288 K and 427 K where the target molecule is completely contributed to HB, see Fig. 1 and Table 1 for details. The B3LYP/6-311++G** calculations at 0 K yield that the energy of octameric cluster obtained from the coordinates at 288 K is 16.42 kCal/mol less than that of the cluster at 427 K. EFG tensor calculations were performed for either crystalline monomer or crystalline octameric cluster of α-glycine at two temperatures. Tables 2 and 3 exhibit converted C_Q and η_Q of ^{17}O, ^{14}N and ^{2}H nuclei in monomer and the target molecule in cluster α-glycine, see Eqs. (1) and (2). The available experimental data of C_Q and η_Q for ^{17}O and ^{14}N were also added to Table 2 [28,29]. A quick look at

Table 1
Distances (Å) and angles of C–H...O and N–H...O hydrogen bonds in α-glycine octamer crystal structure at 288 K and 427 K

r [target...neighbor][a]	288 K	427 K	∠[N–H...O][a]	288 K	427 K
O1–2...H1–1	1.729	1.722	N1–1–H1–1...O1–2	169.28	168.36
O1–7...H3–1	2.363	2.343	N1–1–H2–1...O2–8	168.81	167.85
O2–8...H2–1	1.820	1.848	N1–1–H3–1...O1–7	114.92	118.21
O2–6...H3–1	2.102	2.215	N1–1–H3–1...O2–6	154.27	152.56
O1–1...H1–5	1.729	1.722	N1–5–H1–5...O1–1	169.28	168.36
O2–1...H2–4	1.820	1.848	N1–6–H3–6...O2–1	154.72	152.56
O2–1...H5–5	2.920	2.932	C1–5–H5–5...O2–1	110.87	110.56
O2–1...H3–6	2.102	2.215	N1–4–H2–4...O2–1	168.81	167.85
O1–3...H5–1	2.911	2.933	C1–1–H5–1...O1–3	165.12	165.11
O1–2...N1–1	2.771	2.775			
O2–8...N1–1	2.848	2.852			
O1–7...N1–1	2.951	2.946			
O2–6...N1–1	3.066	3.130			
O1–1...N1–5	2.771	2.775			
O2–1...N1–6	3.066	3.130			
O2–1...N1–4	2.848	2.852			
C1–1...O1–3	3.971	3.974			
O2–1...C1–5	3.459	3.454			

[a] The first number denotes the atom number and the second one denotes the molecule number as indicated in Fig. 1.

Table 2

The calculated quadrupole coupling constants (C_Q) and asymmetry parameters (η_Q) of ^{17}O and ^{14}N in α-glycine at 288 K and 427 K

Nucleus	Basis sets	288 K		427 K		Experimental [a]	
		C_Q [b] (MHz)	η_Q [b]	C_Q [b] (MHz)	η_Q [b]	C_Q (MHz)	η_Q
O(1)	6-311+G*	7.48 (7.54)	0.55 (0.41)	7.33 (7.46)	0.52 (0.35)	7.60	0.25
	6-311++G**	7.47 (7.52)	0.55 (0.41)	7.31 (7.44)	0.52 (0.35)		
O(2)	6-311+G*	8.14 (8.55)	0.43 (0.35)	8.15 (8.43)	0.42 (0.36)	8.40	0.00
	6-311++G**	8.14 (8.55)	0.43 (0.35)	8.16 (8.44)	0.42 (0.36)		
N(1)	6-311+G*	1.02 (0.51)	0.34 (0.68)	1.03 (0.66)	0.32 (0.32)	1.18	0.54
	6-311++G**	1.12 (0.47)	0.32 (0.46)	1.13 (0.63)	0.31 (0.18)		

[a] The experimental values are from [28] and [29] for ^{17}O and ^{14}N, respectively.

[b] The calculated results out of parentheses are for monomer molecule, and those in parentheses are for the target molecule in octameric cluster.

the results reveals that the calculated parameters C_Q and η_Q, do not show any significant difference at two temperatures. The following text discusses the calculated EFG results of ^{17}O, ^{14}N and ^{2}H nuclei at the level of B3LYP/6-311++G**.

3.1. ^{17}O EFG tensors

In this section the calculated C_Q and η_Q values of terminal carboxylic group oxygen nuclei, O1 and O2, are discussed, see Table 2. To compare the HB effects on ^{17}O EFG tensors, the calculation were performed for monomer and octameric cluster of α-glycine. The ^{17}O C_Q and η_Q results reveal that O1 and O2 have not identical chemical environments in α-glycine. For both temperatures, 288 K and 427 K, $C_Q(^{17}\mathrm{O1})$ is 1 MHz greater than $C_Q(^{17}\mathrm{O2})$ while the difference between the two nuclei η_Q is almost negligible. The results of Table 2 show that $C_Q(^{17}\mathrm{O2})$ undergoes more reduction than $C_Q(^{17}\mathrm{O1})$ because of contribution to stronger HB crystalline cluster. Fig. 1 illustrates that the carboxylic group of the target molecule in cluster of α-glycine interacts with three neighboring molecules. O1 contributes to one N–H...O═C HB whereas O2 contributes to one C–H...O═C and two N–H...O═C HBs. $C_Q(^{17}\mathrm{O2})$ reduces 0.41 MHz and 0.28 MHz from monomer to the target molecule in cluster at 288 K and 427 K, respectively. On the other hand, $C_Q(^{17}\mathrm{O1})$ reduces 0.05 MHz and 0.13 MHz from monomer to the target molecule in cluster at 288 K and 427 K, respectively, which is less significant than the reduction of $C_Q(^{17}\mathrm{O2})$. This trend reveals the major role of O2 in contribution to HB while that of O1 is minor.

3.2. ^{14}N EFG tensors

In this section, the calculated ^{14}N C_Q and η_Q parameters for monomer and the target molecule in octameric cluster of α-glycine are discussed, see Table 2. Two purposes are aimed in this discussion: first, to investigate the HB effects on the EFG tensors at the site of nitrogen nucleus and second, to compare the calculated results with experimental data. A quick look at the results reveals the discrepancy between experimental and calculated $C_Q(^{14}\mathrm{N})$ results of monomer at both temperatures. However, when HB effects are considered in the cluster, a good agreement is observed between experimental and calculated $C_Q(^{14}\mathrm{N})$ results. As shown in Fig. 1, $^{+}\mathrm{NH}_3$ terminal site of the target molecule in octameric cluster of α-glycine interacts with four neighboring molecules through four N–H...O═C HB, $r_{\mathrm{N1-1...O1-2}}=2.771$ Å, $r_{\mathrm{N1-1...O1-7}}=2.951$ Å, $r_{\mathrm{N1-1...O2-8}}=2.848$ Å, $r_{\mathrm{N1-1...O2-6}}=3.066$ Å.

The calculated $C_Q(^{14}\mathrm{N})$ values of the target molecules at 288 and 427 K are 1.12 and 1.13 MHz, respectively, which are in good agreement with the experimental value at 287 K, $C_Q(^{14}\mathrm{N})=1.18$ MHz [29]. Because of HB effects, $C_Q(^{14}\mathrm{N})$ increases 0.65 MHz and 0.50 MHz from monomer to the target molecule in octameric cluster at 288 and 427 K, respectively. HB also influence on the $\eta_Q(^{14}\mathrm{N})$ of the target

Table 3

The calculated quadrupole coupling constants (C_Q) and asymmetry parameters (η_Q) of ^{2}H in α-glycine at 288 K and 427 K

Nucleus	Basis sets	288 K		427 K	
		C_Q [a] (MHz)	η_Q [a]	C_Q [a] (MHz)	η_Q [a]
H(1)	6-311+G*	162.75 (186.79)	0.02 (0.01)	146.27 (170.15)	0.02 (0.01)
	6-311++G**	166.06 (194.57)	0.02 (0.01)	148.79 (177.30)	0.02 (0.01)
H(2)	6-311+G*	172.85 (201.33)	0.02 (0.05)	203.19 (231.48)	0.02 (0.05)
	6-311++G**	178.60 (206.09)	0.01 (0.05)	210.22 (240.12)	0.02 (0.04)
H(3)	6-311+G*	196.69 (212.38)	0.01 (0.03)	262.31 (276.33)	0.01 (0.03)
	6-311++G**	203.98 (220.53)	0.02 (0.03)	271.31 (286.01)	0.01 (0.03)
H(4)	6-311+G*	195.74 (193.11)	0.08 (0.10)	198.26 (195.68)	0.08 (0.10)
	6-311++G**	201.39 (198.94)	0.09 (0.10)	203.97 (201.58)	0.08 (0.10)
H(5)	6-311+G*	191.10, 198.69	0.09 (0.10)	214.85 (222.20)	0.09 (0.09)
	6-311++G**	196.69 (204.55)	0.09 (0.10)	220.81 (228.43)	0.09 (0.09)

[a] The calculated results out of parentheses are for monomer molecule, and those in parentheses are for the target molecule in octameric cluster.

molecule where the calculated results are in good agreement with the experiment.

3.3. ^2H EFG tensors

In two previous sections, the influence of HB on the EFG tensors at the sites of oxygen and nitrogen nuclei has been discussed. The results of Table 3 also reveal the influence of HB on the EFG tensors at the sites of hydrogen nuclei in the cluster. For the target molecule, three hydrogen nuclei of $^+NH_3$ contribute to N–H...O═C HB and one hydrogen of >CH_2 (H5) contributes to C–H...O═C HB in octameric cluster, see Fig. 1. $C_Q(^2H1)$, $C_Q(^2H2)$ and $C_Q(^2H3)$ reduce 28, 30 and 16 kHz, respectively, from monomer to the target molecules at both temperatures. On the other hand, because of C–H...O═C HB, $C_Q(^2H5)$ reduces 7 kHz from monomer to the target molecule. Since hydrogen nuclei have poor electronic environments, the changes of η_Q are almost negligible in the cluster of α-glycine.

4. Conclusion

The preceding work performed DFT calculations of ^{17}O, ^{14}N and ^2H EFG tensors in the α-glycine crystalline structures at 288 and 427 K. The comparison of the calculated results of monomer and the target molecule in octameric cluster reveal the influence of N–H...O═C and C–H...O═C HB types on the EFG tensors at the sites of ^{17}O, ^{14}N and ^2H nuclei in the crystalline structure of α-glycine. Since the octameric cluster includes all possible contributions to HB for the target molecule, the calculated EFG results of ^{14}N are in good agreement with the experiments. For oxygen nuclei, O2 has the major role of contribution to HB whereas that of O1 is minor. Among the hydrogen nuclei, HB has the remarkable influence on the EFG tensors at the site of H2.

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