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A systematic study on hydrogen bonding interaction between formamide and cytosine

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ABSTRACT

A systematic computational study was carried out to characterize the hydrogen bonding of complexes formed between formamide and cytosine by DFT calculations. The computations were performed mainly with the B3LYP/6-311++G(d,p) level. Seven stable cyclic structures are found on the potential energy surface, in which four structures have two normal hydrogen bonds and the others have only one normal hydrogen bond with a very weak hydrogen bond that can be neglected. In the four structures with two normal hydrogen bonds, two have seven-membered rings, and the others have an eight-membered ring. The eight-membered ring is preferred to the seven-membered one by analyzing the hydrogen bond lengths and the interaction energies. The infrared spectrum frequencies, vibrational frequency shifts and charge number are also reported.

1. Introduction

It is important that DNA(RNA) should interact with proteins [1–3], which are fundamental materials in the structure of most living things and play a variety of structural and functional roles in all biological systems, to replicate themselves and characterize the information encoded in genes. For transcription and DNA replication, enzymes should be bound to DNA and copy the DNA base sequence sequentially. For information characterization, transfer RNA(tRNA) should interact with amino acids to form aminoacyl tRNA and then construct expected proteins. So it is worthwhile to investigate interactions between DNA and proteins. Among so-called protein–nucleic acid interactions, the hydrogen (H)-bonding are mainly electrostatic in character.

It is an interesting subject to investigate the effects of long-range interactions such as hydrogen bonding because of the unique role in chemical and biochemical systems, especially the contribution to the stability and conformational variability of nucleic acids. Understanding the nature of these interactions can be crucial in describing the function of these systems in biological media at the molecular level. A proper description of these non-bonded interactions helps to understand the basic principles governing the formation of the 3D nucleic acid architectures, nanoarchitectures of nucleic acids [4] and [5]. In many cases, the type of these hydrogen bonding is N–H...O and N–H...N which is mainly electrostatic with some charge transfer and polarization in nature. Due to the importance, there has been extensively investigated by either experimental or theoretical studies up to now [6–12].

The geometric constraints of the amide bond, such as the nearly planar structure around the C–N bond because of its partial double-bond character, define the conformational freedom of motion for many small molecules as well as for peptides and proteins. Formamide that is usually chosen as the backbone of proteins to study the biological systems exhibiting the peptide type of bonding complex and hydrogen-bond interactions [13–19] has been selected at present. As a matter of fact, numerous experimental and theoretical studies have been reported that formamide complexes such as formamide–water and formamide–methanol can serve as model systems for protein–water and protein–solvent interactions. Cytosine is not only a pyrimidine base and a constituent of nucleotides but also one of important components of DNA, which is the origin of life. In fact, cytosine can exist in other non-canonical tautomeric forms from proton transfer reactions. Some of the tautomeric forms may cause the base mispair, which has been proven to be one of the origins of gene mutation [20]. Because of its great importance in chemistry and biology sciences, many studies of cytosine have been reported in the past. Early in 1998, Mikael Pera1kyla1 reported the pK_a of cytosine N3 [21]. The electron correlation of cytosine has been studied by Géza Fogarasi [22]. Lishan Yao et al. have investigated the catalytic mechanism of yeast cytosine deaminase [23]. Bernhard Lippert and Jerzy Leszczynski have discussed the complex of cytosine and metal ion [24]. As one of important components of DNA, the complex of cytosine and peptides or proteins is no doubt of great significance in chemistry and biology. In the current work, a systematic

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investigation of the characteristics of H-bond between formamide and cystine is carried out on model structures, selecting different H-bond-sites among the monomers and considering all the possible combinations of geometrical features.

2. Computational methods

It is well known that in the SCF model, the electrostatic exchange and some induction–polarization effects are included. In more recent years, it has been learned that the induced–induced dispersion interaction may be of great importance [25]. Therefore it is necessary to go beyond the SCF model and include some of the correlation effects. Ab initio calculations have been performed with wave functions based density functional theory methods (DFT) at 6-311++G(d,p) basis set and second-order Moller–Plesset perturbation theory (MP2) at 6-31G basis set. The choice of these basis sets is based on the consideration that, in order to obtain reliable properties of hydrogen-bonded complexes, the addition of polarization and diffuse functions to the basis set is necessary.

The geometric optimization of the monomers (formamide and cytosine) and the structures of the formamide–cytosine complexes have been fully optimized by B3LYP at 6-311++G(d,p) basis set and MP2 at 6-31G basis set. The harmonic frequencies and infrared intensities have been calculated at the same level of theory. The formamide–cytosine binding energy has been calculated as the difference between the energy of the complex and the sum of the energies of the separated monomers. The counterpoise procedure of Boys and Bernardi [26] has been applied to correct the basis set superposition error (BSSE). All calculations are performed using the Gaussian 98 program [27].

3. Results and discussion

3.1. Geometries

The fully optimized geometries for the formamide–cytosine complexes and monomers are shown in Fig 1. The geometry parameters of formamide and cytosine monomer, and formamide–cytosine complexes are listed in Table 1 and Table 2.

The calculated results gained by B3LYP/6-311++G(d,p) show that the changes of the geometry upon complexation are relatively minor. For formamide in Table 1, the maximum bond length change is C14N16 bond which changed from 1.3603 Å in formamide to 1.3303 Å in FC5. The others changes are less than 0.02 Å, while the maximum change of C14O15 is 0.0172 Å from 1.2120 Å in formamide to 1.1948 Å in FC6. And the maximum change of C14N17 is 0.0192 Å from formamide to FC7, while the maximum bond changes of N16H18 and N16H19 are 0.015 Å and 0.174 Å, respectively. The same is true in cytosine, except the C5N7 bond, which maximum change is 0.0397 Å from FC6 to cytosine, namely it shortens, and the other bond length changes can also be neglected. The C3N8 bond length shortens by 0.0247 Å from cytosine to FC7, while the C3N4 bond length undulates from 1.2969 Å to 1.3302 Å in the complexes. The changes of the three NH bonds in cytosine are especially minor, and none of them is larger than 0.015 Å. This may be due to the stable six-membered ring structure in cytosine.

In the seven optimized complexes, four of them are cyclic, with two hydrogen bonds in the interaction, which are FC1, FC4, FC5 and FC7 as can be seen in Fig. 1. As to structures FC2, FC3 and FC6, there are also two hydrogen bonds in the interaction, but one of the bonds is too weak (the bond length are nearly 3.0 Å and even 3.9 Å) to be considered as a normal hydrogen bond, as shown in Table 2.

In FC1, the O15 and N4 act as proton acceptors, while H13 and H18 act as proton donors. Two strong hydrogen bonds are formed between O15 and H13, and between N4 and H18. The bond lengths are 1.854 Å and 1.949 Å respectively, and the bond angles are 178° and 168°. Because of the formation of hydrogen bond of O15H13, the N8H13 bond and C14O15 double bond weaken slightly, while the N8H13 lengthens from 1.0070 Å in cytosine to 1.0275 Å in FC1, and the C14O15 double bond lengthens by 0.0177 Å from formamide to FC1. The affinity of C14 to O15 weakens as the bond length of C14O15 lengthens, so the affinities of C14 to H17 and N16 become stronger, and the bond lengths of C14H17 and C14N16 are slightly shorter in the FC1 than in formamide. Meanwhile the N16H18 lengthens by 0.234 Å from 1.0066 Å in cytosine to 1.0300 Å in FC1 due to the effect of hydrogen bond of N4H18. Connected with the two hydrogen bonds, an eight-membered ring emerges in the complex, from which we can suppose that large interaction energy will be gained. The structure of FC7 is similar to FC1 as the formamide monomer is in the same region of cytosine. Different from the structure of FC1, in FC7 the formamide is transverse, and the eight-membered ring is replaced by a seven-membered ring. The two hydrogen bonds in FC7 are formed between O15 and H13, and between N4 and H17. With a large tensile force of the seven-membered ring, the hydrogen bonds in FC7 are not as strong as in FC1. The bond lengths and bond angles are 2.022 Å and 2.478 Å, 169° and 133°, respectively.

The mechanisms of FC4 and FC5 are very similar to FC1 and FC7.

As for the structures of FC2, FC3 and FC6, we consider that each of them has only one hydrogen bond while the other hydrogen bond is too weak. In structure FC2, the acceptors of proton are O6 and N4, and the donors are H17 and H19. The hydrogen bond formed between O6 and H19 has a bond length of 1.956 Å and

Table 1
Geometrical parameters of cytosine, formamide and seven complexes (length in Å) at B3LYP/6-311++G(d,p) level.

		FC1	FC2	FC3	FC4	FC5	FC6	FC7
Cytosine								
N8H12	1.0043	1.0054	1.0048	1.0047	0.991	0.9907	0.9952	0.9905
N8H13	1.007	1.0275	1.008	1.0075	0.9935	0.9932	0.9926	1.0026
C3N8	1.3582	1.3429	1.3534	1.3541	1.3498	1.3468	1.3374	1.3335
C3N4	1.3173	1.3302	1.3217	1.3214	1.2969	1.2992	1.3001	1.3039
N4C5	1.3689	1.3654	1.3617	1.3621	1.3594	1.3548	1.3578	1.3553
C5O6	1.2161	1.2205	1.2252	1.2248	1.2008	1.2058	1.1956	1.1973
C5N7	1.4283	1.4198	1.4163	1.4165	1.3929	1.3886	1.4009	1.3986
N7H11	1.01	1.0097	1.0102	1.0103	1.0044	1.0054	0.9938	0.994
Formamide								
C14O15	1.212	1.2297	1.2201	1.2193	1.2015	1.2039	1.1948	1.2006
C14N16	1.3603	1.3395	1.351	1.3507	1.3415	1.3303	1.3411	1.3432
C14H17	1.106	1.1036	1.1046	1.1061	1.0871	1.0912	1.0909	1.0868
N16H18	1.0066	1.03	1.009	1.009	0.9942	0.9916	0.9946	0.994
N16H19	1.0091	1.0071	1.0184	1.0184	0.9917	1.0058	0.9919	0.9917

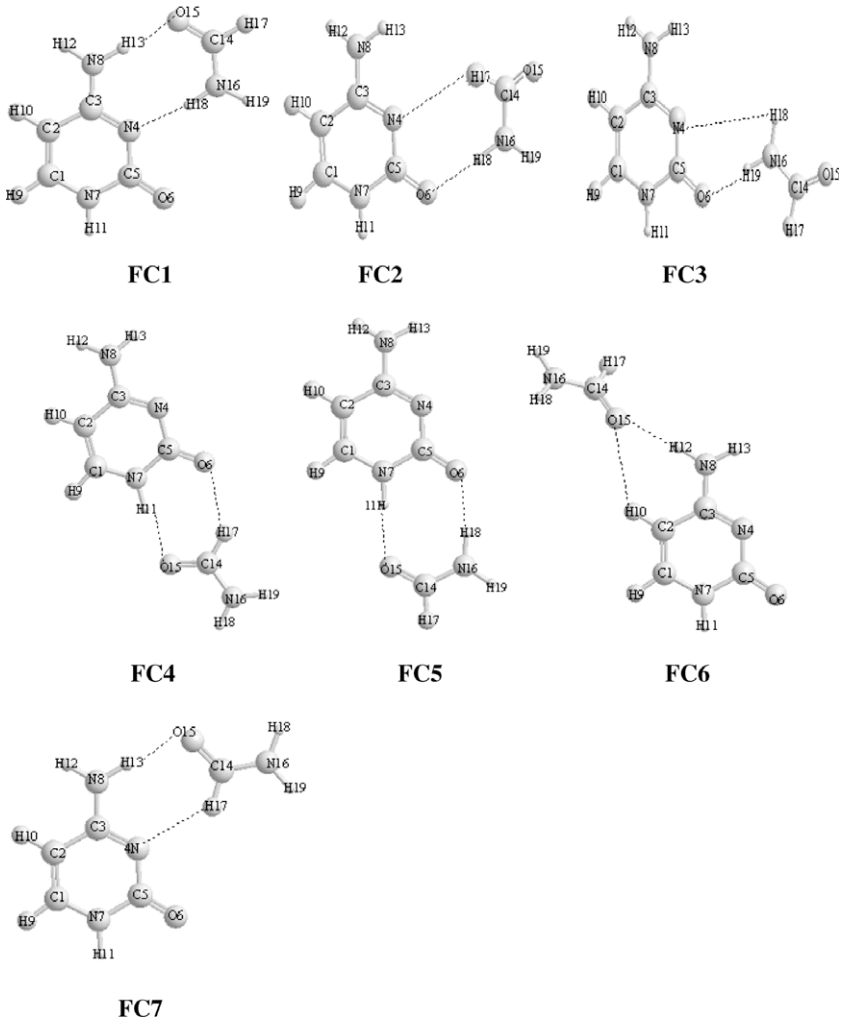

Fig. 1. Optimized structures of formamide–cytosine complexes at B3LYP/6-311++G(d,p) level.

Table 2
Optimized hydrogen bonds of the formamide–cytosine complexes at B3LYP/6-311++G(d,p) level.

	Bond lengths (Å)		Bond angles (deg.)	
FC1	O15 H13 = 1.854	N4H18 = 1.949	N8H13O15 = 178	N4H18N16 = 168
FC2	O6H19 = 1.956	N4H17 = 2.904	N4H17C14 = 133	O6H18N16 = 177
FC3	O6H19 = 1.941	N4H18 = 3.953	O6H19N16 = 178	
FC4	O15H11 = 1.960	O6H17 = 2.368	N7H11O15 = 170	C14H17O6 = 134
FC5	O15H11 = 1.939	O6H18 = 1.957	N7H11O15 = 176	N16H18O6 = 167
FC6	O15H12 = 2.101	O15H10 = 2.980	O15H12N8 = 172	O15H10C2 = 131
FC7	O15H13 = 2.022	N4H17 = 2.478	N8H13O15 = 169	N4H17C14 = 133

bond angle of 177°, which is acceptable. However the hydrogen bond length of N4H17 is 2.904 Å, and it is so large that the interaction of N4 and H17 can be neglected. Due to the effect of the O6H19, the C5O6 double bond is prolonged from 1.2161 Å in cytosine to 1.2252 Å in the structure of FC2, and the N16H19 also lengthens from 1.0091 Å to 1.0184 Å. The bond length of C14H17 nearly remains the same from formamide monomer to FC2, namely is only prolonged by 0.0014 Å, which can also indicate that the interaction of N4 and H17 can be neglected. For the structure of FC3, the hydrogen bond between H18 and N4 in fact is inexistent as the bond length is large to 3.953 Å, far beyond the normal hydrogen length. In FC6, the acceptor of proton is O15, and the donors are H10 and H12. O15 forms two hydrogen bonds with H10 and H12 simultaneously. The O15H12 has a normal hydrogen bond length of 2.101 Å and a bond angle of 172°. The interaction of O15 and H10 is very unnoticeable due to the large bond length of O15H10 of 2.980 Å.

3.2. Binding energies

The energy of binding cytosine to formamide molecule has been determined by:

$$E_{\text{int}} = E_{\text{cytosine–formamide}} - E_{\text{cytosine}} - E_{\text{formamide}} \quad (1)$$

where E_{cytosine}, $E_{\text{formamide}}$ and $E_{\text{cytosine–formamide}}$ are the electronic energies of cytosine, formamide and the complex system, respectively. For the result gained by MP2 method, to correct the basis set superposition error (BSSE), the counterpoise (CP) method is employed. In this case, the corrected E_{int} is given by:

$$E_{\text{int(cp)}} = E_{\text{cytosine–formamide}} - E_{\text{cytosine(cp)}} - E_{\text{formamide(cp)}} \quad (2)$$

where $E_{\text{cytosine(cp)}}$ and $E_{\text{formamide(cp)}}$ are computed with the basis set of the complex FC.

To analyze the role of basis set size effects on the binding energy between formamide and cytosine, we show all the results in Table 3, which gives a detailed analysis of the binding energy obtained with several different theoretical models. The numbers shown in the parenthesis gained by MP2 are corrected for BSSE using the counterpoise method of Boys and Bernardi.

Table 3
Interaction energies (kJ/mol) of formamide–cytosine complexes at B3LYP/6-311++G(d,p) level.

	B3LYP/6-311++G(d,p)	MP2/6-31G
FC1	65.22	79.42 (73.38)
FC2	37.67	50.96 (44.64)
FC3	36.2	48.66 (43.00)
FC4	45.67	56.62 (50.98)
FC5	69.47	82.03 (76.34)
FC6	27.95	36.54 (30.45)
FC7	42.54	53.00 (46.68)

From the values presented in Table 3, it can be seen that the relative stability order of the seven structures is FC5, FC1, FC4, FC7, FC2, FC3, FC6, and the orders of the seven structures gained by the two different methods are well consilient. It is easy to understand that the structures of FC5, FC1, FC4 and FC7 are more stable than the other three structures as they all have a pair of hydrogen bonds between formamide and cytosine. The structures of FC5 and FC1 process an eight-membered ring while FC4 and FC7 process a seven-membered ring. Because the tensile force is not so strong in an eight-membered ring as in a seven-membered one, so the stability of FC5 and FC1 is better than FC4 and FC7. As to FC6, besides the weak interaction, the formamide molecule and cytosine are not in the same plane as the other structures are, so the FC6 is the most unstable structure in the seven complexes.

3.3. Frequencies and charge numbers

The harmonic vibrational frequencies of the seven optimized complexes and the monomers calculated by B3LYP/6-311++G(d,p) are listed in Table 4. Charge numbers of seven conformers of the formamide–cytosine complexes are also calculated with B3LYP/6-311++G(d,p) level, as shown in Table 5.

The strongest vibrational mode is the asymmetrical stretch of NH2 group. In the structures of FC1, FC2, FC3 and FC5, the N16H18H19 asymmetrical stretch red-shifts distinctly, while in the structures of FC4, FC6 and FC7 the change is unconspicuous (3957.9 cm^{-1}, 3954.8 cm^{-1} and 3958.6 cm^{-1}). As we can see from Fig. 1, the hydrogen bond unformed in the NH2 group of FC4, FC6 and FC7. That is to say, the hydrogen bond formation has effect to the vibration of relative group or atom. The N16H18H19 symmetrical stretch vibration has the similar trend. The C14H17 stretch vibration blue-shifts by 84.3 cm^{-1} and 87.4 cm^{-1} in the FC4 and FC7, respectively, as the result of a strong hydrogen bond. The others change slightly, especially the FC3, where there are not any hydrogen bond on O15 or H17 atoms. The stretch of C14O15 double bond gets a red-shift markedly to 1886.2 cm^{-1} in FC4 from 1956.4 cm^{-1} in formamide. The changes of the N8H12H13 stretch are not as evident as the others in the process except in FC1, FC6 and FC7, whose hydrogen bond unformed in NH2 group of cytosine. As to the intensity of C7H11, it changes greatly from 3870.6 cm^{-1} in the free cytosine to 3685.6 cm^{-1} in FC4, corresponding to red-shift. The changes of the stretching frequencies of C5O6 double bond are very similar to the changes of C14O15. In a word, the stretch frequencies in complexes associated with the hydrogen bond shift greatly compared with the free monomer.

Table 5 shows the clear charge numbers of the seven complexes as well as the monomer. From Table 5, we can see that the charge numbers of each atoms change greatly in the complexes compared with them in monomers due to the effect of the formation of hydrogen bond. The largest changes appear in the atom with which a hydrogen bond is formed. Generally speaking, without the effect of other atoms the stronger the hydrogen bond is, the larger the charge number change, for example the charge number of O6 is −0.379 in FC2 and −0.382 in FC3, respectively, and the hydrogen bond O6H19 in FC2 is 0.015 Å longer than it in FC3. When the other atoms which have nothing to do with the hydrogen bond are considered, the rule will be broken. For example, though the hydrogen bond occurred on O15 in FC1 is 0.106 Å shorter than that in FC4, the charge number of O15 in FC1 is 0.073 lower than that in FC4 because of the affinity of H17.

4. Conclusions

The hydrogen-bond interaction of the complexes between formamide and cytosine has been analyzed using B3LYP and MP2 methods. Seven stable cyclic structures are found on the potential energy surface, in which four structures have two normal hydrogen bonds and the others have only one normal hydrogen bond with a very weak hydrogen bond that can be neglected. In the four structures with two normal hydrogen bonds, two are seven-membered rings and the others are eight-membered rings. The eight-membered ring is preferred to the seven-membered one by analyzing the hydrogen bond lengths and the interaction energies. Of them, FC5 is the most stable structure, and FC6 is the most unstable one as it has only one hydrogen bond and the noncoplanar structure. The infrared spectrum frequencies, vibrational frequency shifts and charge numbers are also reported. We have found that the stretching frequency associated with the hydrogen bond undergoes a greater shift than the free monomer and there is an extremely large increase in the intensity of the stretching vibration of the hydrogen donor.

Table 4
Selected frequencies of the monomers and complexes at B3LYP/6-311++G(d,p) level.

Freq.	Assignment	FC1	FC2	FC3	FC4	FC5	FC6	FC7
Formamide								
3959	N16H18H19 as-stretch	3924.7	3917	3914.9	3957.9	3922.7	3954.8	3958.6
3817.4	N16H18H19 stretch	3665.7	3754	3749.7	3817.8	3645.8	3814.9	3818.4
3158.8	C14H17 stretch	3169.3	3187	3159.4	3243.1	3178.2	3185.3	3246.2
1956.4	C14O15 stretch	1927.9	1929.8	1930.8	1886.2	1915.4	1934.2	1901.1
1765.9	N16H18H19 scissors	1778.8	1790.5	1792.9	1766.1	1786.2	1769.3	1765.1
1199.7	N8H12H13 rock in plane	1230	1214.4	1205.3	1215.5	1190	1224.1	1226.4
Cytosine								
3977	N8H12H13 as-stretch	3935	3971.9	3973.3	3962.1	3967.5	3941.8	3939
3870.6	C7H11 stretch	3873.2	3867.3	3866.9	3685.6	3674.4	3876.5	3873.9
3835.8	N8H12H13 stretch	3690.7	3832.3	3833.4	3827.7	3830.8	3794.2	3697
1935.9	C5O6 stretch	1900.6	1902.3	1904.7	1918	1883.3	1920.1	1917.3
1778.6	N8H12H13 scissors	1832.3	1782.8	1781.9	1780.4	1778.9	1801.3	1806.7
1199.7	N8H12H13 rock	1230	1214.4	1205.3	1215.5	1215.72	1224.1	1226.4

Table 5
Charge numbers of monomers and complexes at B3LYP/6-311++G(d,p) level.

	FC1	FC2	FC3	FC4	FC5	FC6	FC7	FA	C
C1	−0.288	−0.165	−0.126	0.040	−0.037	0.004	−0.200	−0.199	
C2	0.330	0.188	0.118	−0.240	−0.170	−0.178	0.010	0.157	
C3	−0.238	−0.171	−0.116	−0.101	0.078	0.144	0.284	−0.138	
N4	−0.364	−0.303	−0.300	−0.510	−0.512	−0486	−0.484	−0.310	
C5	0.242	0.144	0.105	0.430	0.494	0.447	0.456	0.224	
O6	−0.385	−0.379	−0.382	−0.477	−0.513	−0.473	−0.475	−0.360	
N7	−0.301	−0.291	−0.290	−0.505	−0.511	−0.501	−0.483	−0.304	
N8	−0.416	−0.296	−0.283	−0.399	−0.409	−0571	−0.590	−0.303	
H9	0.165	0.179	0.182	0.193	0.199	0.209	0.205	0.160	
H10	0.182	0.186	0.183	0.216	0.229	0.238	0.214	0.174	
H11	0.335	0.334	0.334	0.539	0.507	0.369	0.376	0.328	
H12	0.266	0.276	0.277	0.279	0.288	0.445	0.395	0.269	
H13	0.383	0.297	0.290	0.309	0.314	0.322	0.441	0.292	
C14	0.301	0.022	0.086	0.150	0.299	0.283	0.048		0.114
O15	−0.444	−0.372	−0.389	−0.517	−0.541	−0.537	−0.517		−0.370
N16	−0.455	−0.437	−0.437	−402	−0614	−0.436	−0.385		−0.336
H17	0.104	0.121	0.078	0.211	0.140	0.123	0.328		0.078
H18	0.500	0.399	0.420	0.298	0.447	0.293	0.285		0.247
H19	0.281	0.267	0.250	0.283	0.292	0.292	0.272		0.266

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