

N-甲替甲酰胺-水的氢键团簇的从头计算研究*

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摘要: 利用从头计算方法在 MP2/6-31 + G** 和 MP2/6-311 ++ G(d, p) 水平上对 N-甲替甲酰胺(NMF)-水氢键团簇进行了研究. 计算给出了所有中性和离子化 NMF-H₂O 团簇的优化结构、解离通道以及解离能. 对于 N-甲替甲酰胺, 顺式结构比反式结构具有更低的能量. 对于质子化的 NMF, 质子倾向于连接在甲替甲酰胺的氧原子上. 计算结果表明, NMF 的顺式和反式构型都可以与水分子形成线型的氢键结构. 尽管 NMF 反式结构比顺式结构能量高, 但由于反式结构能与水分子形成双氢键, 因此能更稳定的存在. N-甲替甲酰胺-水团簇电离后, 无论顺式和反式结构均有质子化产物生成.

关键词: N-甲替甲酰胺-水团簇; 从头计算研究; 质子转移

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Ab initio Study of the Hydrogen-bonded Clusters of N-methylformamide-water*

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Abstract The N-methylformamide(NMF)-water clusters were studied by *ab initio* calculations at MP2/6-31 + G** and MP2/6-311 ++ G(d, p) levels. The equilibrium geometries and the dissociation channels and dissociation energies of both neutral and ionic NMF-H₂O clusters are presented. For N-methylformamide, *cis*-form has lower energy than *trans*-form. In NMFH⁺, the proton prefers to link with the O atom of N-methylformamide. The results show that both *cis*- and *trans*- form of NMF can form a linear hydrogen bond with water. Although the energy of *trans*-NMF is higher than *cis*-NMF, *trans*-form exists more stably because it can form a double hydrogen bond with water. After the ionization of the NMF-H₂O cluster, both the *cis*- and the *trans*-form will produce protonated products.

Keywords NMF-water clusters, *ab initio* calculations, Proton transfer

1 Introduction

The proton transfer through hydrogen bonding has attracted much attention because it is an important mechanism of many chemical and biological processes^[1-3]. It has been found that in the ionization

process of many hydrogen-bonded clusters, the predominant products are protonated ones. These protonated products are suggested to arise from an intracuster proton transfer reaction accompanying the dissociation processes^[4-6].

The research about the structure of N-methyl-

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formamide (NMF) is a very interesting subject for biochemistry scientists^[7], because NMF is the simplest molecule that consists of a functional group $-\text{CO}-\text{NH}$ responsible for nucleic base pairing in DNA, and it is a simplest model to understand the properties of peptide-bond containing material, such as the proton transfer in protein and the hydrolysis of the peptide bond in biological systems. NMF can be used as a drug combined with ultrasound to kill cultured HL-60 human promyelocytic leukemia cells^[8], which also plays an important role in eradication of tumors because it has an antitumor activity^[9]. A lot of experimental studies have been performed on the N-methylformamide molecule, such as synchrotron radiation^[10], infrared spectroscopy^[11], electron diffraction^[12], low wave number vibrational spectra^[13], nuclear magnetic resonance (NMR)^[14], microwave spectrum^[15] and Rydberg electron transfer spectroscopy^[16] etc. Also theoretical calculations^[17-21], Monte Carlo^[22] and molecular dynamics simulations^[23] have been carried out for NMF. For the understanding of the structural properties and biological functions of amides and proteins, it is important to know how they interact with solvents, and particularly with water. The Raman spectra of the C=O stretching mode of N-methylformamide mixed with various solvents were systematically studied as a function of concentration^[24]. Complexes formed between fluorobenzene and N-methylformamide^[25], N-methylformamide + water^[26], N-methylformamide + ethanol^[27], formamide + N-methylformamide binary mixture^[28] were studied.

In this work, we carry out *ab initio* studies of NMF-water clusters, present geometry structures and the proton transfer through hydrogen bonding of NMF-water clusters.

2 Methods of calculation

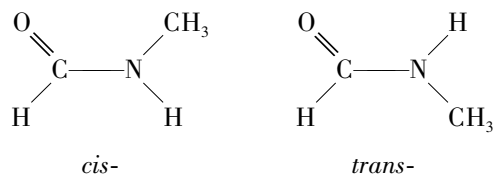
The program Gaussian 98^[29] was used in the computations. Geometric optimization of all the molecules and clusters were evaluated at MP2/6-31 + G (d , p) level. The harmonic vibrational frequencies have been calculated at this level to confirm the stationary points, which were also used to consider the zero-point energy

(ZPE). MP2/6-311 ++ G (d , p) single-point calculations were performed on the final optimized structure. For the dissociation energy of the neutral NMF-H₂O cluster, the basis set superposition error (BSSE) correction was carried out using the counterpoise (CP) method. Since the value of s^2 is close to the ideal value 0.75, spin contamination was negligible. To give a comparison, some energy calculations were also carried out at B3LYP/6-311 + G (2df 2p) level.

3 Results and discussion

3.1 The structure and the protonation of NMF

The electronic ground state of NMF is $(1a')^2 \dots (13a')^2 (1a')^2 (2a')^2 (3a')^2$ ^[30]. According to the relative location relationship of methyl and carbonyl, this molecule may have two stable geometries: *cis*-form and *trans*-form, as shown in the figure below:



In the study of rotational spectrum of NMF, Fantoni and Caminati considered that the *cis*-form is more stable than *trans*-form^[15]. The structure of $-\text{CO}-\text{NH}$ group of NMF is planar, just like the geometry of peptide.

The equilibrium structures and parameters of NMF and NMF⁺ at the MP2/6-31 + G (d , p) level are shown in Fig. 1, and the corresponding energies are given in Table 1. We can see that NMF has C_s symmetry as shown in Fig. 1 a and b. The present calculated results are in satisfactory agreement with other experiments and calculations^[12 21 31]. As shown in Table 1, the energy of *trans*-form is about 4 kJ/mol less stable than *cis*-form, which means that a relative concentration of the *trans*-form NMF is 15% ~ 10%, and that is in good agreement with the experimental data at a temperature of -15°C ^[15]. Because the C₁-N bond has the properties analogous to a double bond, and its rotation energy barrier is 63 ~ 84 kJ/mol which is higher than the typical single bond, *cis*- and *trans*-structure can't be exchanged from one into another through a ro-

tation of the single bond.

Ionic NMF^+ also has the *cis*- and *trans*- structures as shown in Fig. 1c and d. Compared with the neutral NMF, in the *cis*- NMF^+ the $\text{C}_1 - \text{N}$ bond decreases by 0.06 \AA , but $\text{C}_1 - \text{O}$ bond and $\text{N} - \text{C}_2$ bond increase by 0.06 and 0.025 \AA respectively. Although O, C_1 and N atoms are located still in the same plane, the H_2 atom is bent out of the plane, and the H_3 and H_5 atoms of methyl are no longer symmetrical. In the *trans*-form, the $\text{N} - \text{C}_1$ bond increases by 0.2 \AA , but the $\text{C}_1 - \text{O}$ bond and $\text{N} - \text{C}_2$ bond decrease by 0.08 and 0.02 \AA respectively. It can be seen from the Mulliken popula-

tion of atomic charges that the ionization of *cis*-NMF may take place in the N atom. This is the reason why the $\text{N} - \text{C}_1$ bond is contracted. And the *trans*-NMF may be ionized in O atom, it causes weaken of the $\text{C}_1 - \text{O}$ bond and strengthen of the $\text{N} - \text{C}_1$ bond. The energy of the *cis*-form is lower than the *trans*-form and about 15 kJ/mol .

Protonation plays an important catalytic role in amido bond hydrolysis^[32]. There are two plausible protonation sites of the amide in the acid-catalyzed hydrolysis mechanism: the protonation occurs on either oxygen or nitrogen. Cho *et al.* studied the protonation of

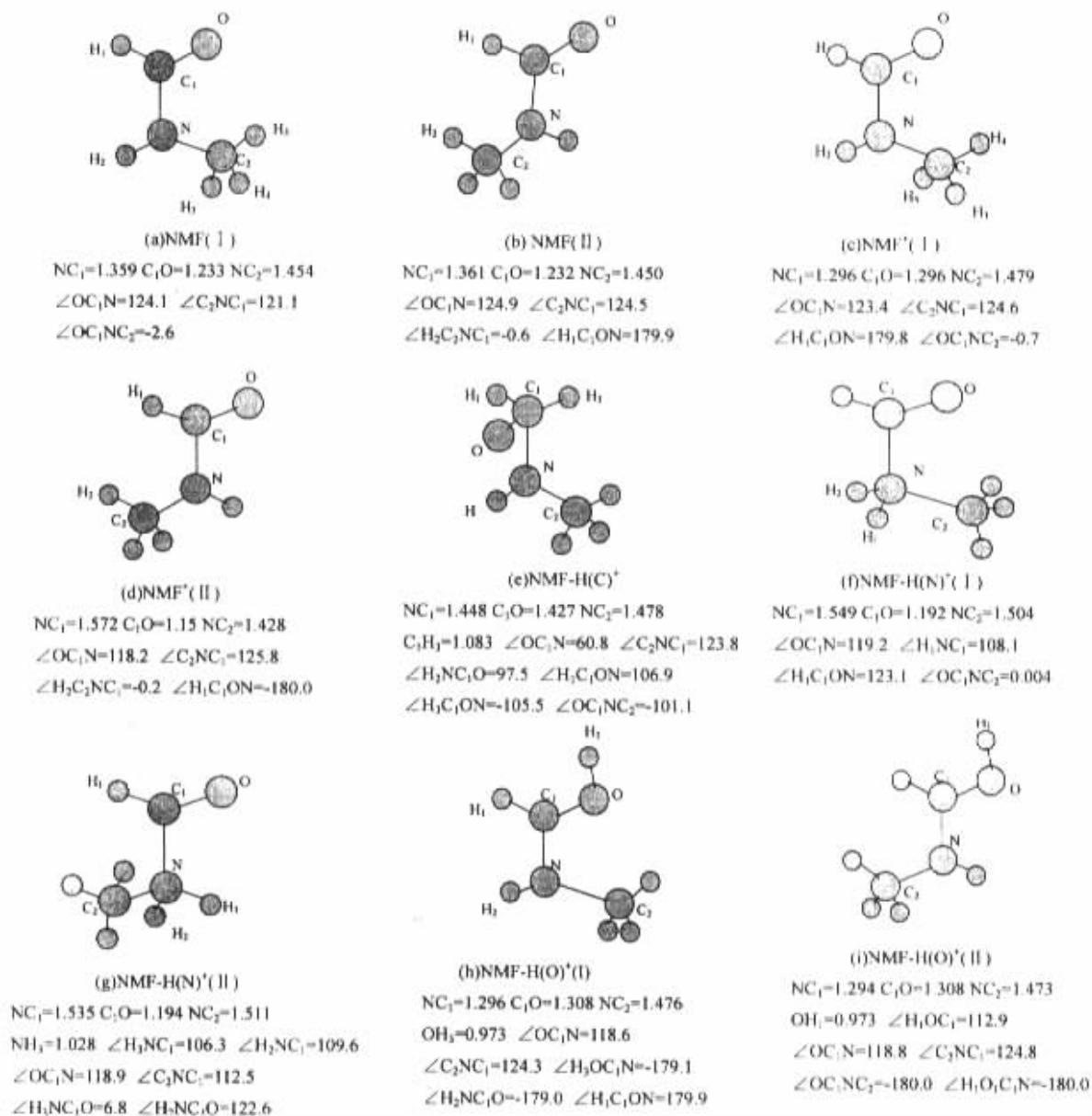


Fig. 1 Geometries of NMF monomer and protonated NMF calculated at MP2/6-31 + G** level

Table 1 Calculated total energy and zero-point vibrational energy of NMF ,
NMFH⁺ and NMF-H₂O binary clusters (Unit : Hartree)

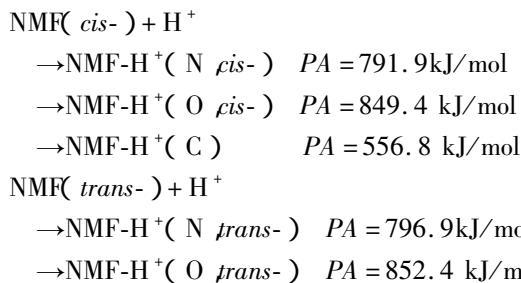
Species	B3LYP ^a	S ²	ZPE	MP2 ^b	S ²	ZPE	Ref.[19]
NMF(<i>cis</i> -)	-209.2843204	—	0.074161	-208.6920416	—	0.075559	-208.6551850
NMF(<i>trans</i> -)	-209.2826629	—	0.074094	-208.6896794	—	0.075691	-208.6530175
NMF ⁺ (<i>cis</i> -)	-208.925152	0.777	0.070985	-208.3277238	0.761	0.075915	-208.6556631
NMF ⁺ (<i>trans</i> -)	-208.9253281	0.780	0.071373	-208.3203892	0.846	0.074131	-208.6534220
NMF-H ⁺ (C)	-209.5095439	—	0.087639	-208.9184624	—	0.089708	
NMF-H ⁺ (N χ I)	-209.5930175	—	0.087423	-209.0075454	—	0.089151	
NMF-H ⁺ (N χ II)	-209.5921933	—	0.087391	-209.0069268	—	0.089110	
NMF-H ⁺ (O χ I)	-209.6241048	—	0.088135	-209.0301948	—	0.089865	
NMF-H ⁺ (O χ II)	-209.6231481	—	0.087925	-209.0287087	—	0.089755	
NMF-H ₂ O(I)	-285.7540472	—	0.097434	-284.9769624	—	0.099563	
NMF-H ₂ O(II)	-285.7570142	—	0.098440	-284.9780769	—	0.100335	
NMF-H ₂ O(III)	-285.7555057	—	0.098469	-284.9758367	—	0.100496	
NMF-H ₂ O(IV)	-285.757268	—	0.098550	-284.9788221	—	0.100485	
NMF-H ₂ O(V)	-285.7596004	—	0.099324	-284.9806866	—	0.101532	
NMF-H ₂ O ⁺ (I)	-285.4193123	0.773	0.095233	-284.6307439	0.854	0.099117	
NMF-H ₂ O ⁺ (II)	-285.4131114	0.755	0.097140	-284.6203393	0.834	0.099143	
NMF-H ₂ O ⁺ (III)	-285.4177624	0.774	0.094896	-284.6286026	0.871	0.098053	
NMF-H ₂ O ⁺ (IV)	—	—	—	-284.6262389	0.818	0.100241	

a. B3LYP/6-311 + ζ (2df,2p) // B3LYP/6-31 + ζ (d,p) values. b. MP2/6-311 ++ ζ (d,p) // MP2/6-31 + ζ (d,p) values.

formamide and its substituent products by using *ab initio* calculation^[33]. They concluded that O-protonation (a proton is linked to O atom of formamide) was favored than N-protonation.

Ab initio calculations were performed on the protonated NMF by present work , and five equilibrium structures were obtained based on a geometry optimization , which are shown in Fig. 1 e ~ i. Both O-protonation and N-protonation NMF have two structures : *cis*- and *trans*-forms. As shown in Table 1 , the energies of *cis*-forms are lower than *trans*-forms too. From the structure parameters we can see that , when a proton is linked with the O atom , the C₁ - O bond lengthens about 0.08 Å , but the N - C₁ bond decreases by about 0.06 Å. However when a proton is linked with N atom , the N - C₁ bond is lengthened by about 0.2 Å , but the C₁ - O bond is shortened by about 0.04 Å. The reason is that when protonation occurs at O atom , the C₁ - O bond has the characteristics of a single bond , while the C₁ - N bond has the characteristics of

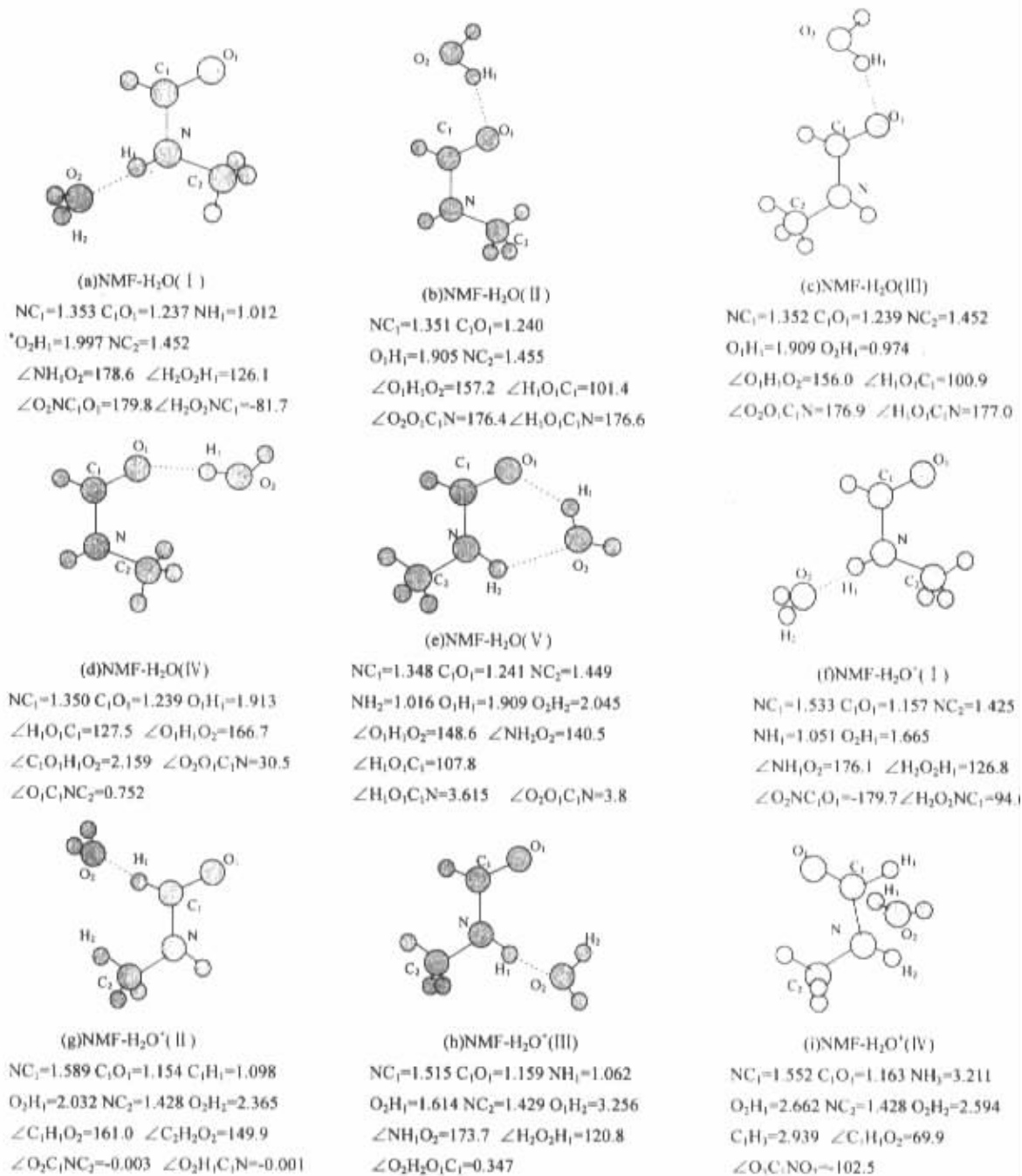
a double bond. For the C-protonation NMF , both N - C₁ bond and C₁ - O bond are lengthened. From the energies listed in Table 1 , we can achieve proton affinities (PA) of these three positions as follows :



In good accord with Cho , the O atom is the best proton acceptor in the protonated NMF. And the present values of PA (849.4 and 852.4 kJ/mol) are consistent with the reference result (851.3 kJ/mol)^[34]. It can be seen that the calculation results obtained at the present level of theory are reasonable.

3.2 The structures of neutral and ionic NMF-H₂O clusters

Fig. 2 depicts the calculated equilibrium structures

Fig. 2 Geometries of NMF-H₂O cluster calculated with MP2/6-31 + G** method

and parameters of both neutral and ionic NMF-H₂O clusters at the MP2/6-31 + G** level.

As can be seen from Fig. 2a, a linear hydrogen bond N...H₁-O₂ is formed between the neutral NMF and H₂O molecules, where NMF is a proton donor. The O atom of H₂O is located in the plane of NMF, and the two H atoms of H₂O are located symmetrically on both sides of this plane. Fig. 2 b and c show that

the *cis*- and *trans*-form NMF can be linked to H₂O via the hydrogen bonds respectively, where the molecules H₂O are the proton donors. And the H₂O and the C₁, O₁, N atoms of NMF are located nearly in a plane. The energy of the *cis*- structure is lower than the *trans*-structure. In Fig. 2d *cis*-NMF and H₂O form a cluster with a hydrogen bond O₁...H₁-O₂, where the molecule NMF is a proton acceptor, and H₂O is a proton

donor. The cluster of NMF(*trans*-)-H₂O can be found in Fig. 2e , and the C = O bond and N - H bond are in a plane. Two hydrogen bonds of O₁...H₁-O₂ and N...H₂-O₂ can be formed between the *trans*-NMF and H₂O molecules. The double hydrogen bonding structure is similar to that of formamide-H₂O binary cluster^[35]. It can be known from the energy listed in the Table 1 that the structure (V) of NMF(*trans*-)-H₂O clusters is more stable than the other four structures.

For the ionic NMF-H₂O cluster , four equilibrium structures can be obtained based on a geometry optimization. As shown in Fig. 2f , the structure of ionic type (I) is analogous to the neutral structure (I) , but the distance between O₂ and H₁ decreases by 0.33 Å , mainly due to a stronger electrostatic interaction in the ions. It can be seen from Fig. 2 g and h that structure (II) and (III) are the complexes of *trans*-NMF and H₂O. In the structure (II) a ring structure can be constructed from the O₂ atom of H₂O and the H₁ , H₂

atoms of the NMF. The two atoms of H₂O are located symmetrically on both sides of the ring. In a linear hydrogen bond of the structure (III) , the H atom is linked to the N atom of NMF and the molecule H₂O is a proton acceptor. The two hydrogen atoms of H₂O are laid at a plane , which is constructed from C₁ , O₁ and N atoms of NMF. For the structure (IV) given in Fig. 2i , the O₂ atom of water molecule and the H₁ and H₂ atoms of NMF can form a ring analogous to structure (II). From the energies given in Table 1 , it can be known that the ionic cluster NMF-H₂O (I) has lowest energy among the ionic clusters of NMF-H₂O. Thus , it can be deduced that the most stable configuration of ionic NMF-H₂O should be the structure (I).

3.3 Ionization , dissociation and proton transfer reactions of NMF-H₂O cluster

The calculated energy changes of reactions for NMF-H₂O binary cluster system are summarized in Table 2. From the dissociation energy after BSSE

Table 2 Summary of the reaction energies for NMF-H₂O cluster system^a

1	NMF(<i>cis</i> -)→NMF ⁺ (<i>cis</i> -) + e	IP = 956.5 kJ/mol
2	NMF(<i>trans</i> -)→NMF ⁺ (<i>trans</i> -) + e	IP = 964.6 kJ/mol
3	NMF-H ₂ O(II)→NMF(<i>cis</i> -) + H ₂ O	D ₀ = 21.3 kJ/mol(23.8 kJ/mol _{BSSE})
4	NMF-H ₂ O(V)→NMF(<i>trans</i> -) + H ₂ O	D ₀ = 31.5 kJ/mol(33.7 kJ/mol _{BSSE}) ^c
5	NMF-H ₂ O(I)→ NMF-H ₂ O ⁺ (I) + e	IP = 907.0 kJ/mol
6	NMF-H ₂ O(V)→ NMF-H ₂ O ⁺ (III) + e	IP = 914.4 kJ/mol
7	→ NMF-H ₂ O ⁺ _{verb} + e	IP _{verb} = 998.6 kJ/mol
8	NMF-H ₂ O ⁺ (I)→ NMF ⁺ (<i>cis</i> -) + H ₂ O	D ₀ = 70.0 kJ/mol
9	→ NMF-H ⁺ (N , <i>cis</i> -) + OH	D ₀ = 110.3 kJ/mol
10	→ NMF-H ⁺ (O , <i>cis</i> -) + OH	D ₀ = 52.8 kJ/mol
11	→ NMF-H ⁺ (C) + OH	D ₀ = 345.5 kJ/mol
12	NMF-H ₂ O ⁺ (II)→ NMF ⁺ (<i>trans</i> -) + H ₂ O	D ₀ = 57.2 kJ/mol
13	NMF-H ₂ O ⁺ (III)→ NMF ⁺ (<i>trans</i> -) + H ₂ O	D ₀ = 81.7 kJ/mol
14	→ NMF-H ⁺ (N , <i>trans</i> -) + OH	D ₀ = 109.0 kJ/mol
15	→ NMF-H ⁺ (O , <i>trans</i> -) + OH	D ₀ = 53.6 kJ/mol
16	NMF-H ₂ O ⁺ (IV)→ NMF ⁺ (<i>cis</i> -) + H ₂ O	D ₀ = 55.2 kJ/mol
17	→ NMF-H ⁺ (N , <i>cis</i> -) + OH	D ₀ = 95.6 kJ/mol
18	→ NMF-H ⁺ (O , <i>cis</i> -) + OH	D ₀ = 38.0 kJ/mol
19	→ NMF-H ⁺ (C) + OH	D ₀ = 330.7 kJ/mol

a. MP2/6-311 ++ G(d , p)/MP2/6-31 + G(d , p) + ZPE values.

b. The subscript ver indicates vertical ionization.

c. BSSE indicates BSSE error corrected.

correction of the NMF-H₂O cluster given in Table 2 , it can be known that the BSSE error is not significant in this basis set.

As shown in Table 2 , the ionization potential (IP) value of neutral NMF-H₂O cluster is 907 kJ/mol , which is red-shifted about 50 kJ/mol than the NMF monomer. The dissociation energy of reaction 4 is 31.5 kJ/mol , which is higher than that of reaction 3 , because the double hydrogen bonding makes the cluster of NMF(*trans*-)-H₂O more stable than NMF(*cis*-)-H₂O cluster. The ionic cluster NMF-H₂O⁺(I) has four dissociation channels as shown in Table 2. One of the channels can produce an unprotonated NMF⁺ and the others produce the protonated products NMF-H⁺ where protons are linked to N , O or C atoms of NMF respectively. The channel corresponding to produce NMF⁺(O , *cis*-) + OH is the best energy favored , which means that the dominant products are protonated ones after the dissociation of NMF-H₂O⁺(I). The calculation also shows that the ionic cluster NMF-H₂O⁺(III) can dissociate to produce protonated NMF-H⁺(O , *trans*-) and OH through reaction 16 which is energetically favored.

In our rescent paper the formation mechanisms of protonated products via photoionization of some hydrogen-bonded clusters were reported^[36]. To elucidate the reaction mechanism of intracuster proton transfer after cluster photoionization , an *ab initio* calculation of simplified reaction path potential was performed on the optimized structures of NMF-H₂O with MP2/6-311 ++ G (d , p) methods. As shown in Fig. 2e , the hydrogen bond O₁...H₁—O₂ is obviously bent. Analogous to the model^[37] for bent hydrogen systems , during the calculations the hydrogen bond length(the sum of the actual O₁ - H₁ distance and H₁ - O₂ distance) is fixed at the optimized value 2.88 Å. And the optimized distance of O₁ - O₂ is also fixed to be the optimized value 2.79 Å. Relative to the C , N , O heavy atoms , the movement of the lighter bridging H atom should be much faster. Thus , the heavy atoms could be considered to be stationary. For other H atoms in H₂O and NMF , their effects on the bridging hydrogen are neglected , due to that the positions of these atoms in their ionic cluster

shift very little related to the neutral one , as shown in Fig. 2. According to the above hypothesis , the potential energy cures of the neutral NMF-H₂O (V) cluster and its ionic cluster are calculated based on MP2/6-311 ++ G (d , p) level with the bridging hydrogen moving across toward the O₂ atom in step (step size is 0.05 Å). It shows that for the neutral cluster , as shown in Fig. 3 curve n , the bridging H atom tends to be closer to the O₂ atom than the O₁ atom. After vertical ionization , the bridging H atom prefers to move to O₁ atom (as shown in Fig. 3 curve m). It can be understandable that when NMF-H₂O (V) is vertically ionized (*IP*_{ver} = 998.6 kJ/mol) , a surplus energy may be enough to make the ionic cluster dissociate into NMF⁺(O , *cis*-) and OH. Thus , it can be expected that for NMF-H₂O cluster , the measured ions after ionization should be a sequence of protonated product.

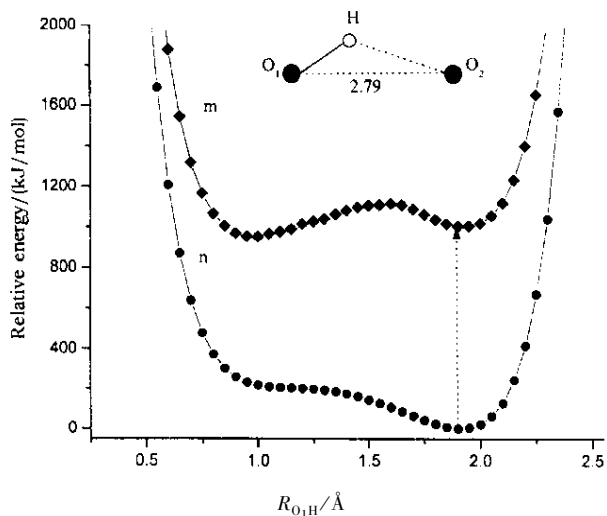


Fig. 3 Potential energy curve n and vertical ionization potential curve m of the neutral NMF-H₂O cluster calculated at MP2/6-311 ++ G (d , p) level. *R*_{O₁H} is the distance between the O₁ and H atom

4 Conclusions

The NMF-H₂O binary cluster was studied by *ab initio* calculations. For N-methylformamide , *cis*-form has lower energy than *trans*-form. In NMFH⁺ , the proton prefers to link with the O atom of N-methylformamide. The results show that both the *cis*- and *trans*-NMF can form a linear hydrogen bond with H₂O. The energy of *trans*-NMF is higher than that of *cis*-

form, but it can form double hydrogen bond with H_2O , and therefore, the corresponding NMF- H_2O cluster can exist more stable. After the ionization, the dominant dissociation channels of *cis*- and *trans*-isomers are the same, *cis*-form primarily produces protonated products NMF- $H^+(O_{cis-})$ and OH, and the dominant products of *trans*-form are protonated products NMF- $H^+(O_{trans-})$ and OH.

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