

# THEORETICAL STUDY ON THE INTERMOLECULAR INTERACTIONS OF 1,1-DIAMINO-2,2-DINITROETHYLENE WITH NH<sub>3</sub> AND H<sub>2</sub>O

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**Abstract**—Density Functional Theory (DFT) and dispersion-corrected density functional theory (DFT-D) were used to study the intermolecular interactions of 1,1-diamino-2,2-dinitroethylene FOX-7/NH<sub>3</sub> and FOX-7/H<sub>2</sub>O supermolecules. The geometries optimized from DFT and DFT-D methods are similar.

Six optimized supermolecules were characterized to be local energy minima on potential energy surfaces without imaginary frequencies. The intermolecular interaction energy (binding energy) was calculated with basis set superposition error (BSSE) correction. The largest corrected intermolecular interaction energy is FOX-7/NH<sub>3</sub> (-43.76 kJ mol<sup>-1</sup>), indicating that the interaction between FOX-7 and NH<sub>3</sub> is stronger than that of FOX-7/H<sub>2</sub>O. The same conclusion is obtained from the studies on the infrared spectrum and frontier orbitals.

These instructions are presented to assist authors in preparing a typescript which is suitable for direct photo-offset reproduction. The abstract should not exceed 200, 150 and 50 words for Review Papers, Articles and Notes respectively.

**Keywords**—1,1-diamino-2,2-dinitroethylene; Ammonia; Water; Intermolecular interaction; Theoretical study.

## I. INTRODUCTION

FOX-7 (1,1-diamino-2,2-dinitroethylene) is a novel nitramine explosive and an ingredient in solid propellants (Anniyappan *et al.*, 2006; Gerardo *et al.*, 2007) with high thermal stability and low sensitivity to impact and friction. Since the successful synthesis of FOX-7 (Latypov *et al.*, 1998), its performance has attracted many researchers attention in the field of energetic materials (Asta and Lou, 1999; Ou and Liu 2005).

Previous studies on FOX-7 have mainly been focused on density, reactivity, thermal stability, compatibility, sensitivity, specific heat capacity and so on. Intermolecular interactions, i.e., hydrogen bonding and van der Waals interactions, have become more and more important in modern research (Weber *et al.*, 2011; Alkorta, 2011; Alkorta *et al.*, 1998; Alkorta and Elguero, 1999; Alkorta *et al.*, 2001; Hedgeland *et al.*, 2011; Hursthouse *et al.*, 2011; Xu *et al.*, 2011; Arunan *et al.*, 2011a; Arunan *et al.*, 2011b; Li *et al.*, 2011; Bakulin *et al.*, 2011; Contreras-García *et al.*, 2011; Stiopkin *et al.*, 2011; Alkorta *et al.*, 2006; Rozas *et al.*, 2000; González *et al.*, 1997; Sanz *et al.*, 2008; Mó *et al.*, 1992; Grabowski, 2001a;

Grabowski, 2001b). These interactions are becoming a hot topic especially in condensed matter physics as well as in biology and chemistry (Kaur and Khanna, 2011; Vaupel *et al.*, 2006; Sponer *et al.*, 2013). Among all the intermolecular interactions, the strongest interaction is hydrogen bonding, and a lot of studies have been performed to characterize the nature of hydrogen bonding using different computational methods (Chaudhari *et al.*, 2011; Otaki and Ando, 2011; Zierkiewicz *et al.*, 2010; Truchon *et al.*, 2010; Czyznikowska *et al.*, 2009; Rybalova and Bagryanskaya, 2009; Wheatley and Lillestolen, 2007).

Because DFT method considers electron correlation, its reliability is higher than the HF method. A recent study of large hydrogen-bonded complexes proved the reliability of the DFT-B3LYP method to address hydrogen bonding (Rajeev *et al.*, 2011; Roohi *et al.*, 2011; Szatylowicz and Krygowski, 2010; Roohi *et al.*, 2010).

Understanding the interaction with water or ammonia is of particular importance since the FOX-7 crystal morphology is affected by exposure to water during synthesis or after evacuation. Theoretical study on the intermolecular interactions among FOX-7/NH<sub>3</sub> and FOX-7/H<sub>2</sub>O supermolecules could provide guidelines for the relationship between structure and property of FOX-7 (Sorescu *et al.*, 2001).

Quantum chemistry method has become a powerful method to investigate intermolecular interaction such as hydrogen bond. It is generally accepted that ab initio HF method neglected the electronic correlation energy, thus leading to large errors during structural optimization and energy calculation. MP2 method is not a cost-effective approach for the computation of complicate complexes even with a medium-size basis set. Because DFT method considers electron correlation, its calculation reliability is much higher than HF method. Recently, the B3LYP method of density functional theory has been applied to large H-bonded complexes. It is accepted that for H-bonded complexes, the B3LYP approach yields relatively reliable structures and interaction energies. Therefore, DFT method is an ideal tool for discovering intermolecular weak interactions, which has been proved by the previous work (Roohi *et al.*, 2011).

In this paper, DFT-B3LYP/6-311++G\*\* and DFT-D methods were used to study the intermolecular hydrogen bonding interactions. Because DFT functionals are not always a good approximation and due to the approximate nature of the applied functionals, standard DFT methods often fail catastrophically for energetic crystals. This is

due to the localized nature of density functionals. Sorescu *et al.* performed theoretical predictions for several energetic molecular crystals, and claimed that the dispersion-corrected density functional theory (DFT-D) method as parametrized by Grimme provides significant improvements for the description of intermolecular interactions in molecular crystals at both ambient and high pressures relative to conventional DFT (Grimme, 2006). Thus, DFT-D calculations are also included.

## II. COMPUTATIONAL DETAILS

All structures under DFT method are optimized using Gaussian 03 software (Frisch and Pople, 2003). Normal mode analysis for each structure resulted in no imaginary frequencies, indicating that all structures correspond to the local minima on the potential energy surface. Structure optimizations and vibrational frequency calculations under DFT-D method were performed using Materials Studio version 7.0 (2013).

Interaction energies were estimated from the energy differences between supermolecules and FOX-7. The basis sets commonly used to calculate energies are far from being saturated. As a result, each sub-system in any complex will tend to lower its energy depending on the use of basis set functions of the other sub-system. The energies obtained at equilibrium geometry of complex for each sub-system are lower than those calculated at the same geometry with basis set functions of respective sub-system alone. This energy difference is so-called basis set superposition error (BSSE). The binding energies of the supermolecules are equal to the differences between the supermolecules and the monomers after correcting for the BSSE energies.

## III. RESULTS AND DISCUSSION

Figure 1 lists the optimized geometries under DFT (B3LYP/6-311++G\*\*) and DFT-D levels of the title compounds. I, II and III are the dimers of FOX-7/H<sub>2</sub>O, IV, V and VI are the dimers of FOX-7/NH<sub>3</sub>, VII is the optimized FOX-7. The optimized geometry of FOX-7 is similar with Sorescu *et al.* (2001). We can see that the geometries optimized using DFT and DFT-D are similar, so we can conclude that the DFT method is also suitable for these gas-phase clusters, so the following discussions are all based on the DFT results.

In supermolecule II, there are two hydrogen bonds, the O atoms in nitro group and water molecule are the hydrogen-bond acceptor, hydrogen atom in amino group of FOX-7 and water molecule act as hydrogen-bond donors.

As for supermolecule III, this configuration is consistent with the study by Sun *et al.* (2007), in which two hydrogen bonds are present; (O15-H12 + O15-H14) the O atom in water is the hydrogen-bond acceptor and the two hydrogen atoms in the amino group of FOX-7 act as hydrogen-bond donors.

In the FOX-7/NH<sub>3</sub> dimers, for example for dimer IV, the hydrogen (N15-H14) length is 1.9713 Å and is the smallest among all the hydrogen bonds mentioned in the article, suggesting that dimer IV is the most stable. This will be confirmed by results presented below.

So we can see that among all the supermolecules, IV and V have only one hydrogen bond, while the others have have two hydrogen bonds.

Table 1 shows the geometrical parameters of the 7 title compounds, we can see that:

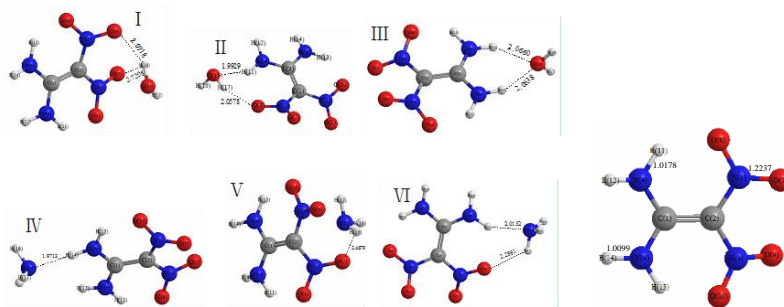


Fig. 1 (a). The optimized geometries of the title compounds and bond lengths (Å) at B3LYP/6-311++G\*\* level.

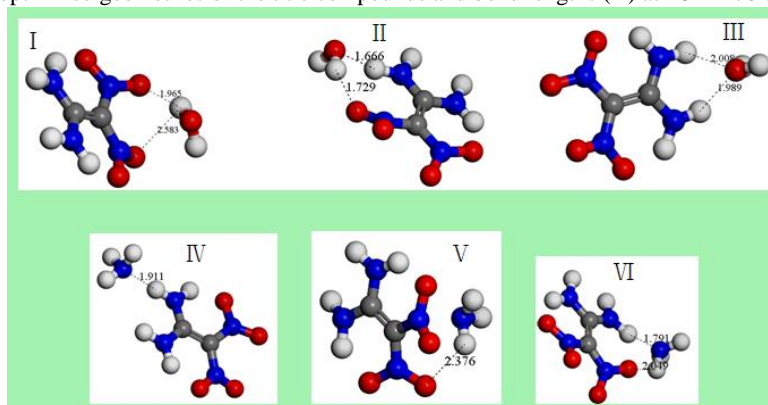


Fig. 1 (b). The optimized geometries of the title compounds and bond lengths (Å) at DFT-D level.

Table 1. Optimized geometries of FOX-7, FOX-7/NH<sub>3</sub> and FOX-7/H<sub>2</sub>O at B3LYP/6-311++G\*\* level (unit: Å)

Bonds	FOX-7	I	II	III	IV	V	VI
N4-H11	1.0178	1.0181	1.0209	1.0147	1.0157	1.0175	1.0175
N5-O7	1.2237	1.2273	1.2237	1.2257	1.2258	1.2285	1.2265
N6-H14	1.0099	1.0099	1.0095	1.0139	1.0280	1.0090	1.0103
N3-O9	1.2237	1.2305	1.2255	1.2257	1.2259	1.2259	1.2257

Table 2. Total energy ( $E_t$ ), corrected energy ( $E_{t,c}$ ) and binding energy at B3LYP/6-311++G\*\* level

supermolecule	$E_t$ (a.u.)	$E_{t,c}$ (a.u.)	BSSE (kJ·mol <sup>-1</sup> )	Binding energy (kJ·mol <sup>-1</sup> )
I	-674.7307	-674.7250	15.06	-13.62
II	-674.7349	-674.7292	14.79	-24.64
III	-674.7395	-674.7363	8.44	-43.11
<b>IV</b>	<b>-654.8778</b>	<b>-654.8755</b>	<b>6.15</b>	<b>-43.76</b>
V	-654.8656	-654.8619	9.81	-8.11
VI	-654.8723	-654.8692	8.35	-27.04
H <sub>2</sub> O	-76.4089	-76.3878		
NH <sub>3</sub>	-56.5479	-56.5134		

(1) The bond length of N4-H11 is 1.0178 Å in monomer molecule FOX-7, the corresponding values are 1.0181, 1.0209, 1.0147, 1.0157, 1.0175 and 1.0175 Å respectively in supermolecules I, II, III, IV, V and VI. So it is elongated slightly.

(2) The bond length of N5-O7 is 1.2237 Å in monomer molecule FOX-7, in the six supermolecules, the corresponding values are 1.2273, 1.2237, 1.2257, 1.2258, 1.2285 and 1.2265 Å respectively, so the elongation of bond N5-O7 is also small.

(3) N3-O9 bond is also elongated slightly from the monomer molecule to the supermolecules.

(4) The bond N6-H14 is elongated 1.8 pm from the monomer molecule to the supermolecule IV and the deviation is the most obvious among all the supermolecules. The influence of intermolecular interaction on bond bending or internal rotation is small, since the bond angles of all supermolecules are changed only slightly with respect to the monomer molecule FOX-7, which is also consistent with the conclusion from the analysis of dihedral angles. Therefore, it can be speculated that among all the supermolecules, the intensities of interactions of IV may be the strongest.

### A. Binding energies

Table 2 and 3 list the total energy ( $E_t$ ), corrected total energy ( $E_{t,c}$ ), BSSE energy and the corrected interaction energies based on B3LYP/6-311++G\*\* and MP2/6-311++G\*\* levels. There are no imaginary frequencies for any structures, indicating that the structures in Fig. 1 indeed represent the minima on their potential energy surfaces. It is imperative to correct both the BSSE and zero point energy (ZPE).

As is shown in Table 2, the BSSE energies are 15.06, 14.79, 8.44, 6.15, 9.81 and 8.35 kJ mol<sup>-1</sup> respectively for the supermolecules I, II, III, IV, V and VI. The BSSE of I and II are similar and larger than for the other supermolecules. The binding energy of IV is the largest (-43.76 kJ mol<sup>-1</sup>), the second is III, the corresponding value is -43.11 kJ mol<sup>-1</sup>.

In the supermolecules between FOX-7 and H<sub>2</sub>O, we can see from Fig. 1 that I has only one hydrogen bond, II

and III have two hydrogen bonds, but the geometry of title compound III is symmetric, the bond lengths of the two hydrogen bonds are almost the same, so its binding energy is the largest. For the interaction between FOX-7 and NH<sub>3</sub>, the bond length of N15-H14 in supermolecule IV is the smallest so it is more stable than the other supermolecules.

From the values of binding energies, it can be deduced that a large proportion of IV might be produced in FOX-7/NH<sub>3</sub> supermolecules, which is consistent with the conclusion from Zhao *et al.* (2012). There is a similarity between dimer III in Zhao's paper and dimer IV in the current paper, in which the hydrogen bonds are all derived from the nitrogen atom in ammonia and the hydrogen atom in the monomer, this order is also consistent with the proposed order based on the geometrical parameters.

Table 3 lists the binding energies calculated from MP2/6-311++G\*\* method, we can see that the results are consistent with the DFT calculation.

We can see that the binding energies for the MP2 calculations (in the Table 2 and 3) are much higher. Previous study in 1994 revealed that DFT calculations underestimate the binding energy of the water dimer (Kim and Jordan, 1994), which is consistent with our research.

### B. Infrared spectrum

The infrared vibrational spectrum is an important property of a monomer and useful experimental tool for the study of supermolecules.

Figure 2 shows calculated IR spectra of FOX-7/NH<sub>3</sub>, FOX-7/H<sub>2</sub>O and FOX-7 obtained at B3LYP/6-311++G\*\* level. Due to the complexity of vibrational modes, it is difficult to assign all the bands. Therefore, only some obvious vibrational modes were analyzed and discussed. On the basis of optimized geometry, vibrational modes and frequencies of the supermolecules and FOX-7 are assigned. For the monomer FOX-7, the band at 1580 cm<sup>-1</sup> corresponds to the symmetric stretch of C1—C2 bond. In the four supermolecules, the bands at 1570 or 1560 cm<sup>-1</sup> also correspond to the symmetric stretches of C1—C2 bond. The main differences between

Table 3. Total energy ( $E_t$ ), corrected energy ( $E_{t,c}$ ) and binding energy at MP2/6-311++G\*\* level

supermolecule	$E_t$ (a.u.)	$E_{t,c c}$ (a.u.)	BSSE (kJ·mol <sup>-1</sup> )	Binding energy (kJ·mol <sup>-1</sup> )
I	-668.5404	-668.5562	41.50	-301.28
II	-668.5422	-668.5653	60.64	-327.32
III	-668.5565	-668.5732	43.77	-345.38
<b>IV</b>	<b>-648.8331</b>	<b>-648.8426</b>	<b>25.15</b>	<b>-379.45</b>
V	-648.8132	-648.8288	40.89	-296.37
VI	-648.8201	-648.8391	50.01	-338.85

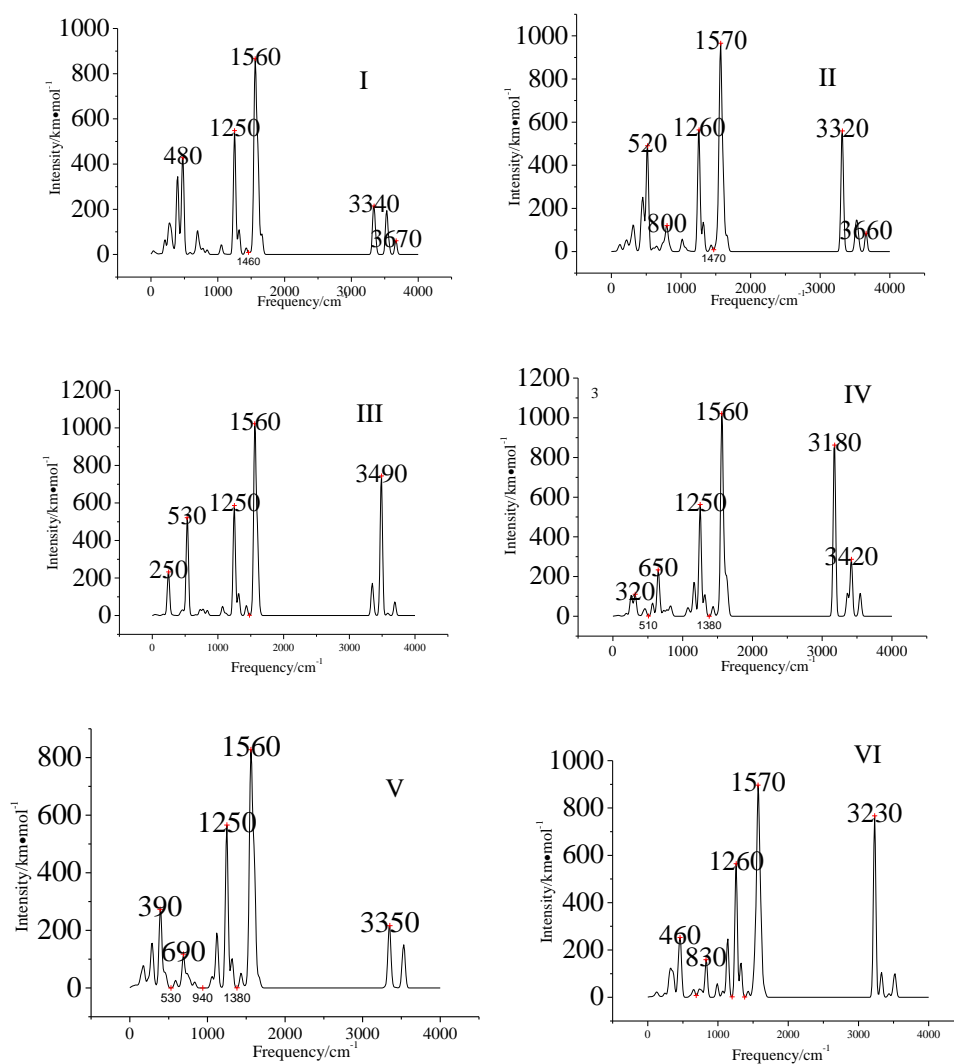


Fig. 2. Calculated infrared spectrum of FOX-7/H<sub>2</sub>O (I, II and III), FOX-7/NH<sub>3</sub> (IV, V and VI) and FOX-7 at B3LYP/6-311++G\*\* level

the FOX-7 and supermolecules are the bands located at higher than 3000 cm<sup>-1</sup>, the bands higher than 3000 cm<sup>-1</sup> are the bonds involving hydrogens. We can see that in FOX-7, the hydrogen bonds' symmetric stretch locate at 3340 cm<sup>-1</sup>, from I to VI, the corresponding shifts are 0, 20, 150, 160, 10 and 110 cm<sup>-1</sup> respectively, and the shifts of IV is highest, which is consistent with the above.

### C. Frontier orbitals

Analysis of the molecular orbitals can provide useful information on electronic structures. Figure 3 lists the highest occupied (HOMO) and lowest unoccupied (LUMO) molecular orbitals of the title compounds. For the title compounds, the skeleton C-N or C-C orbitals participate

in both the HOMO and LUMO levels, and removal of an electron from HOMO level or addition of an electron to the LUMO level could weaken the skeleton framework. We can see that for the supermolecules, the frontier orbitals of IV is almost the same as the FOX-7 while the other supermolecules are somewhat different from the frontier orbitals of FOX-7, which suggests that the formation of IV is preferred from FOX-7.

### D. Thermodynamic Properties

Based on statistical thermodynamics and vibrational analysis, the thermodynamic functions, heat capacities ( $C_p$ ), entropies ( $S^0_T$ ) and thermal correction to enthalpies

( $H_T^0$ ) are obtained from the calculated spectrum (corrected factor 0.96) and are listed in Table 4. From 200 to 800 K, the entropies decrease in the course of the formation dimers from the monomers.

For the dimers of FOX-7/H<sub>2</sub>O, from 200 to 298 K the enthalpies decrease, but when the temperature increases,

higher than 500K, the enthalpies increase, which proves that the formation of FOX-7/H<sub>2</sub>O dimers is automatic when in low temperature but in high temperatures the formation process is forbidden; For the dimers of FOX-7/NH<sub>3</sub>, when the temperature is below 298K, the formation of dimer is favored, while higher than 298K the formation process is forbidden.

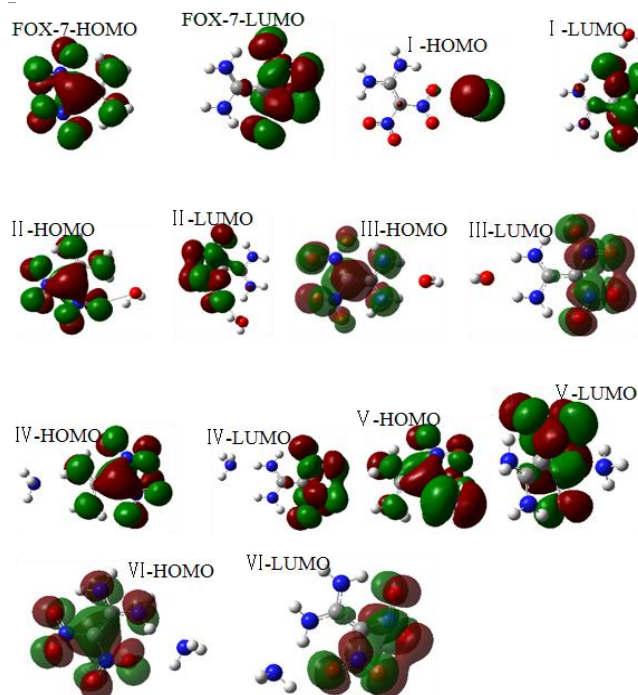


Fig. 3. The HOMO and LUMO frontier orbitals of the title compounds.

Table 4 The thermodynamic properties of dimers at different temperatures under B3LYP/6-311++G\*\* level

Dimers	Temperature K	$C_p$ J/mol/K	$S_T^0$ J/mol/K	$H_T^0$ kJ/mol	$\Delta S$ J/mol/K	$\Delta H$ kJ/mol	$\Delta G$ kJ/mol
FOX-7/H <sub>2</sub> O							
I	200	154.33	400.63	19.09	-119.27	-1.6	22.25
	298.1	196.68	470.51	36.4	-115.35	-0.63	33.76
	500	257.29	587.76	82.71	-108.35	2.13	56.31
	800	308.1	720.98	168.34	-101.06	6.8	87.65
II	200	152.3	401.39	18.9	-118.51	-1.79	21.91
	298.1	194.74	470.46	36.02	-115.4	-1.01	33.39
	500	256.1	586.89	82.02	-109.22	1.44	56.05
	800	307.52	719.7	167.39	-102.34	5.85	87.72
III	200	153.77	408.2	19.47	-111.7	-1.22	21.12
	298.1	195.19	477.62	36.67	-108.24	-0.36	31.91
	500	256.11	594.15	82.69	-101.96	2.11	53.09
	800	307.48	726.94	168.06	-95.1	6.52	82.60
FOX-7/NH <sub>3</sub>							
IV	200	155.48	435.13	20.45	-88.07	-0.25	17.36
	298.1	196.86	505.16	37.8	-84.27	0.69	25.81
	500	261.25	623.27	84.47	-78.08	3.13	42.17
	800	318.53	759.81	172.3	-71.39	7.42	64.53
V	200	160.49	419.34	20.52	-103.86	-0.18	20.59
	298.1	201.34	491.31	38.35	-98.12	1.24	30.49
	500	264.03	611.31	85.74	-90.04	4.4	49.42
	800	319.77	748.78	174.14	-82.42	9.26	75.20
VI	200	155.94	413.32	19.78	-109.88	-0.92	21.06
	298.1	197.98	483.7	37.22	-105.73	0.11	31.63
	500	262.33	602.4	84.13	-98.95	2.79	52.27
	800	319.12	739.34	172.2	-91.86	7.32	80.81

According to the equation  $\Delta G = \Delta H - T\Delta S$ , we can obtain the changes of Gibbs free energies ( $\Delta G$ ) at different temperatures. It is not difficult to find that the sequence of  $\Delta G$  is the same as the  $\Delta H$ , and the value of  $\Delta G$  increases as the temperature increases, thus the interactions are weakened as temperature increases. Since the value of  $H$  is less sensitive to temperature than that of  $T\Delta S$ , the effect of temperature upon  $\Delta G$  is mainly derived from the contributions of the  $T\Delta S$  term for the same dimer. We can see that for the six dimers can be spontaneously produced by a combination of FOX-7 and  $H_2O$  or  $NH_3$  only at low temperatures.

#### IV. CONCLUSIONS

In this paper, DFT and ab initio calculations were performed to study the geometries and intermolecular interaction of FOX-7/ $NH_3$  and FOX-7/ $H_2O$  supermolecules.

Intermolecular hydrogen bonding, damage of conjugated system and directivity of optimized structures play an important role in the stabilization of supermolecules and lead to geometry and electronic structure change. The corrected intermolecular interaction energies were calculated and corresponding interaction intensity for FOX-7/ $NH_3$  is the largest, so the formation of the supermolecule FOX-7/ $NH_3$  is preferred. So during the synthesis, aquated ammonia is favored. The same conclusion is obtained from the studies on the infrared spectrum and frontier orbitals. Thermodynamic analysis showed that FOX-7 and  $H_2O$  or  $NH_3$  dimers are spontaneously produced at temperatures below 298K and are not favorable at temperatures above 298K.

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