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H-bond and conformations of donors and acceptors in model polyether based polyurethanes

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Abstract

The molecular mechanics (MM) method with COMPASS force field was used to study the H-bonds in the polyether based polyurethane model molecules. Availability of the calculation was firstly verified in comparison of some H-bonded model molecules, which were studied by using ab initio calculation, and those calculated by MM. Based on a urethane model molecule 1,3-dimethylcarbamate, which can be donor or acceptor and behaves in various conformations, it is reasonable to have a large number of H-bond interactions between various conformational donors and acceptors. For examining all the possible interaction patterns, we studied 57H-bond complexes. This systematic modeling covers well-known four types of interaction patterns, such as NH···O=C (Type I), NH···O–CO (Type II), NH···NH (Type III), NH···COC (Type IV) in the system. Obtained H-bond energies were used to analyze the probabilities of the complexes. For the interaction within the hard segments, or Type I, Type II and Type III, a predominant H-bond complex has been found in the present study, which belongs to Type I. For the interaction between the hard segment and the soft segment, two conformations of Type IV were calculated to be existed.

Keywords: Hydrogen bond; Molecular mechanics; Polyether based polyurethane

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1. Introduction

Segmented polyurethanes are a type of polymers which consist of the alternating soft and hard segment units. It has been accepted that many of the unusual properties of these materials are primarily due to the two phase structure which is closely related to the relating H-bond [1–4]. H-bond has been an active topic of research for many decades due to its widespread occurrence and importance, and has been investigated by different methods including FTIR [5–8], Raman, X-ray, NMR [9] and quantum chemical calculations [10–17].

The H-bond patterns are different for different polyurethane systems. For polyether based polyurethanes extended by doil, it is widely speculated that there are four types of H-bonding interaction patterns [12,13], since the urethane group [–NH–CO(O)–] provides one H-bond donor and three possible acceptors, and another acceptor of the ether oxygen from soft segments as shown in Fig. 1. The four types of H-bonding patterns are considered to be formed between the NH group and C=O group (Type I), urethane alkoxy oxygen (Type II), NH group (to form NH···NH-bond) (Type III), and ether C–O–C group (Type IV). The first three types deal with the urethane–urethane interaction while the last one concerns the interaction with urethane–soft segment. Of the four, the H-bonds in Type I and IV have been studied in detail [3–8,18,19], especially for the first one. As for Type II, there are arguments with one result showing that the alkoxyl oxygen in the urethane group is not inclined to form the H-bond with N–H [20] while others suggesting such a H-bond is non-negligible [11,12]. There has been no report, however, on Type III.

In the view of H-bonding one may agree with the four types of interaction patters shown in Fig. 1 for the polyether polyurethane system. However, the two bonds, C–N and C–O, at either side of the carbonyl group may have various conformations. As for Type I, Type II and Type III, involving all the conformations of the urethane group, they may have totally 54 different H-bonding configurations. Quantum mechanics (QM) has been used to calculate part of the four H-bonds [10–15] but not present the conclusion

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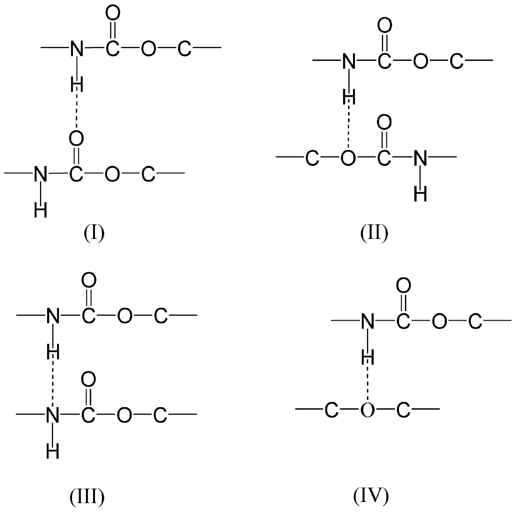


Fig. 1. Four types of H-bonds in polyether based polyurethanes.

concerning all the four types. The above-mentioned conformational effect was not concerned there. Molecular mechanics (MM) is widely accepted as an effectively simpler method compared with QM to obtain reasonable molecular structure and energy. Quality of MM calculation depends on molecular force field. COMPASS force field appeared recently as a high quality force field [21], and is expected to give full play its superiority in simulating these H-bond patterns with various configurations.

Hence in the present work, we report a study on the H-bonding structures with 57 possible configurations in the polyurethane model molecule. According to the calculated energies, the existence possibility of a H-bonding configuration and the probability of various possible interacting configurations were discussed. This study indicates that among the four speculated H-bond types in the polyether based polyurethane Type I and IV are usually observed by means of vibrational spectroscopy.

2. Molecular modeling

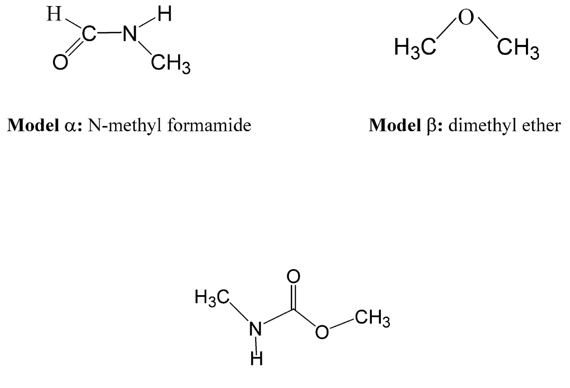
All molecular models were built on Silicon Graphics O_2 workstation using the program Cerius 2 version 3.8 developed by Molecular Simulations Incorporated (MSI). COMPASS [21] force field was used to optimize each model molecule. The high convergence option was adopted for the energy minimization of each model; the root mean square of force on each atom was controlled less than 0.001 kcal mol^{-1} $Å^{-1}$. The basic model molecule is 1,3-dimethylcarbamate. It may have four different conformations. Combining the four conformations, ten different H-bond pairs appear. Taking the first three types of H-bonding interactions as shown in Fig. 1, we calculated 54 different configurations including all the possible H-bonding interaction structures. This calculation deals with individual molecule and molecular complex. For the individual molecule in a conformation, which can be a donor or an acceptor, the energy was obtained after being optimized; whereas for the H-bond complex, the two corresponding molecules were firstly located in a certain position where the H-bond donor atom, H and the acceptor atom are in line with a distance between the donor and the acceptor atom less than 3 Å before optimization. The energy of both the individual donor molecule and the individual acceptor molecule, and the energy of the complex were then obtained. The difference between the sum energy of both individual molecules and the complex energy, ΔE_h, is used as the ‘H-bonding energy’ in the present study.

3. Results and discussion

3.1. Availability of MM in H-bond calculation

The model α and β, dimethyl ether and *N*-methyl formamide, which were used to calculate the H-bonds strength between N–H and C=O as well as N–H and ether by QM [13] were shown in Fig. 2. We firstly verify the availability of MM method using the same molecular models.

Table 1 shows the simulated results including the structure scheme, ΔE_h calculated here by MM and those in the early study by QM. Here we define conformation of the model molecule, and take C=O and CH_3 in the same chain side as *cis*-conformation (*c*). In the QM computations [13], there are different values ΔE_h available from different basis sets. Here listed only are the data on 6-31G Basis Set. We note, however, that there could have different conformations even based on the above two simple model molecules, therefore we just list the energy data based on the same conformations to make the comparison. We have also noted that the different conformations may affect the energy results, which will be discussed below. The data in Table 1 show that the H-bonding energy calculated under COMPASS is quite similar to the results obtained by 6-31G basis



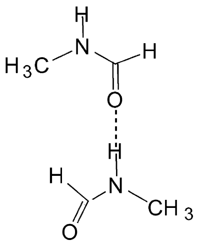
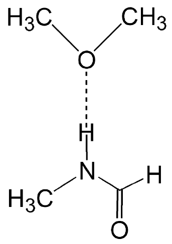
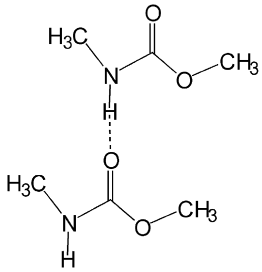
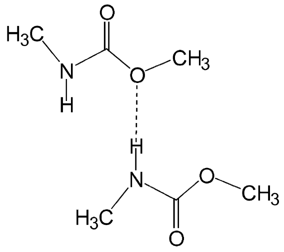
Model α: N-methyl formamide

Model β: dimethyl ether

Model γ: N-methyl methyl carbamate

Fig. 2. The models calculated by QM method: Model α and Model β [13], and Model γ [12].

Table 1
Energy comparison of the H-bond complex calculated by different methods

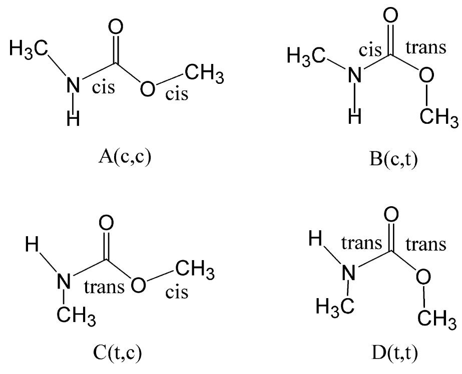
	Structure			
				
Pattern	Type I	Type IV	Type I	Type II
Configuration[a]	$\alpha(c) + \alpha(c)$	$\alpha(c) + \beta$	$\gamma(c) + \gamma(c)$	$\gamma(c) + \gamma(c)$
ΔE_h (kcal mol^{-1}) MM	7.39	5.04	6.88	5.56
ΔE_h (kcal mol^{-1}) QM [13,12]	8.17	5.87	5.03	3.11

[a] $\alpha(c)$ means Model α with *cis* conformation; β stands for Model β; $\gamma(c)$ means Model γ with *cis* conformation.

set of Gaussian package. The first two configurations consist of two Model α or Model α + Model β, and the last two configurations are both comprised of two Model γ (Fig. 2). We still take C=O and CH_3 (attached to alkoxyl oxygen atom) in the same side as *cis*-conformation. Obviously, using different models in calculation of the same configuration, say Type I, one may obtain different values of ΔE_h, such as 8.17 and 5.03 kcal mol^{-1} from QM in the table. Relative to Type I, the COMPASS calculated ΔE_h for Type IV and Type II in reasonable values or orders comparing to those from QM. It suggests that the MM is good in the simulation.

3.2. *Effect of urethane conformations of donors and acceptors on H-bond*

As mentioned above, Model γ has more conformations and is closer to the actual urethane molecules. Therefore we take this model to study the effect of conformations on the H-bonded energy and probability. Since in the model two CH_3 groups attach to either the alkoxyl oxygen atom, or nitrogen atom, one therefore find four possible conformers for Model γ as shown in Fig. 3, namely A(c,c), B(c,t), C(t,c) and D(t,t). The four letters A, B, C, D mean the four conformers, while the two letters c and t, for example c,t in the brackets indicate the local conformation of CH_3 group attached to N in the same side with carbonyl and the one of the other CH_3 group attached to alkoxyl O atom in the opposite side to C=O. Homogeneously, (c,c) means structures around C–N and C–O bond are both in the *cis*-conformation, while (t,t) means the two σ-bond torsions are both in the *trans*-conformation.



A(c,c) B(c,t)
C(t,c) D(t,t)

Fig. 3. Four possible conformers in Model γ.

In energy optimization of the four conformers, we found that D conformer does not exist as it is so unstable that in the optimization (t,t) turns to (t,c) becoming B conformer. Hence there are actually only three conformers, A, B, and C, which would result in six pairs of H-bonded complexes, including A + A, A + B, A + C, B + B, B + C, C + C. Since each of the pairs possibly contains the first three types of H-bonds as shown in Fig. 1, as a result, the six pairs will contain 18 different H-bond configurations (here we define the further possible H-bond pattern in each complex as ‘configuration’ in which the different types of H-bonds are included). Further investigation showed that there are still more H-bond configurations, which are not involved in above sum. This is because when one of the pairs is formed according to Type I, C=O···H–N, only one configuration exists if the donor and the acceptor are the same conformers (say A), (A)C=O···H–N(A), but two configurations exist if the donor and the acceptor are different conformers (say A and B), (A)C=O···H–N(B) and (B)C=O···H–N(A). Therefore, we have not only the three pairs, A + B, A + C and B + C, but also the other opposite three pairs, B + A, C + A and C + B. Hence we now have 9 more H-bond configurations, leading the total different H-bond number up to 27. Furthermore, because various H-bonding groups in the model are not in the central symmetric axis of the molecule, the formed pairs thus possess different conformations when one of the two parts in the pair rotates around H-bond. Here this is recognized as ‘pair conformation’.

Taking this pair conformation into account, if we simply define them as “left” and “right”, there will exist two different pair conformations as shown in Fig. 4, therefore the final total H-bond configuration number will be doubled. It amounts to 54. The above analysis indicates a complexity of H-bond configurations for polyurethane and a shortage of such conformational search in early studies. In the present study, we calculated all the possible H-bond configurations, which belong to the interactions between the hard segments of polyurethane.

Now, we turn our attention to the other interaction system, which is between the soft and the hard segments in polyether based polyurethane. As mentioned above, Type IV describes this interaction as shown in Fig. 1. It is the only type in the polyurethane to form H-bond, which is through Model β and Model γ. Let us count the number of H-bond configurations in such system. Since Model γ, dimethyl ether, does not have different conformations, and only can be the acceptor, and the ether oxygen is in the central symmetric axis, the possible H-bond pairs are three, including A + ether, B + ether, C + ether. Consequently, sum of the configurations from simply the hard segments and the configurations from the soft and the hard segments is 57 in the polyether based polyurethane.

Though many studies concern H-bonds, few of them investigated the effect of the conformations of the donors and acceptors on the H-bond. Even if in the few papers concerning some conformations including using the simulation method [10,12,15,22], the number of conformations investigated there were not complete. Tables 2–4 list the H-bonded energy and probability of 30 different H-bond configurations, which are sorted in three H-bond types and separately in the three tables. It was found in the present study that 24 of the total 54 speculated H-bond configurations could not be formed under the optimization, since they changed themselves into other configurations. The finally formed 30 configurations are distributed in the three types: 18 for Type I, 9 for Type II, and 3 for Type III. The calculation found a reasonable distribution that most H-bonds formed in the optimization have the lengths less than 3.0 Å, and a few have lengths around 3.1 Å.

Table 2 shows that 18 H-bond configurations are in different energies and the lowest energy is -94.953 kcal mol^{-1} in the configuration of $(\mathrm{C}+\mathrm{C})'$. We note that this configuration is a dimer in which two H-bonds form through both NH groups and C=O groups, see Fig. 5.

In order to calculate the probability of each H-bonded configuration, we firstly calculate the statistical weight factor σ_i for each configuration by using Eq. (1), then calculate the partition function Z by using Eq. (2), and finally obtain the probability P_i for each H-bonded complex by

$$\sigma_\mathrm{i} = e^{-\Delta E_\mathrm{i}/RT} \tag{1}$$

$$Z = \sum_i e^{-\Delta E_\mathrm{i}/RT} \tag{2}$$

$$P_\mathrm{i} = \frac{\sigma_\mathrm{i}}{Z} \tag{3}$$

Eq. (3). Where ΔE_i is the energy difference between the energy in each H-bond configuration and the lowest energy -94.953, which we select for the zero point energy. Here RT is simply taken as 600. H-bonded configurations used to make such a calculation for hard segment interactions are shown in Tables 2–4. It is found that the H-bond configuration shown in Fig. 5, (dimer) is predominant, as its probability amounts to almost 95% among all the hard segment H-bonded configurations. The probabilities of other two possible configurations (also dimer) formed from $(\mathrm{A}+\mathrm{A})_{\mathrm{II}}'$ and $(\mathrm{C}+\mathrm{A})_{\mathrm{II}}'$ (Figs. 6 and 7), are only 0.02 and 1.21%, respectively. Table 3 shows that 2 of the 9 Type II H-bonded configurations are relatively stable, yet their probabilities are still very little, only exceeding 1% in the configuration $(\mathrm{C}+\mathrm{A})_{\mathrm{II}}'$, which is a dimer shown in Fig. 7. While Table 4 indicates that NH hardly forms the H-bond with another NH, Type III, since the probability is too little. Although, as Table 4 shows, in the H-bonded complex of $(\mathrm{B}+\mathrm{C})_{\mathrm{III}}$, the H-bond energy is relatively lower, down to -8.34 kcal mol^{-1}, it is actually not caused by Type III H-bond alone, but composed of another H-bond of Type I which results in a H-bond length of 2.918 Å (Fig. 8). Therefore the main energy contribution is obviously from Type I bonding. Even so, its probability is quite little, less than one millionth. This suggests that Type III H-bonds (NH···NH) hardly exist in the system.

Since two different systems were used to study the interaction between the hard segments as well as between the soft and the hard segments, in which the first system consists of two Model γ molecules and the second one a

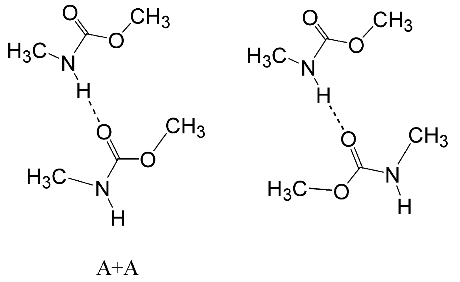


Fig. 4. An example of two different H-bonded types in each H-bonded complex.

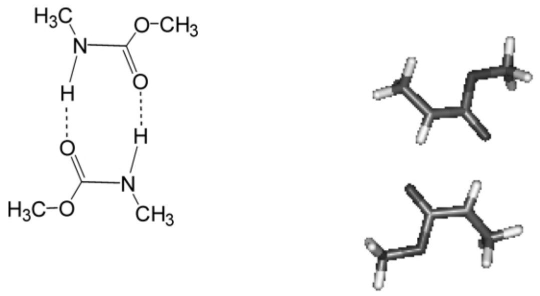


Fig. 5. H-bond dimer formed by Model γ with two C(t,c) conformations.

Table 2
Energy and probability of 18H-bond configurations in Type I

Type	Conformation	H-bond length (Å)	E_{Total} (kcal mol^{-1})	ΔE_h[a] (kcal mol^{-1})	σ (10^{-3})	Probability (%)[b]
$(A + A)_I$	$c,c + c,c$	2.917	−91.041	−6.88	2.8	0.26
$(A + A)_I'$	$c,c + c,c$	2.907	−91.904	−7.74	11.7	1.11
$(A + B)_I$	$c,c + c,t$	2.912	−81.008	−7.81		–
$(A + B)_I'$	$c,c + c,t$	2.909	−80.628	−7.43		–
$(A + C)_I$	$c,c + t,c$	2.924	−90.6550	−6.66	1.5	0.14
$(A + C)_I'$	$c,c + t,c$	2.926	−91.958	−7.96	12.8	1.21
$(B + A)_I$	$c,t + c,c$	2.917	−81.7304	−8.53		–
$(B + A)_I'$	$c,t + c,c$	2.923	−81.3480	−8.15		–
$(B + B)_I$	$c,t + c,t$	2.935	−70.526	−8.29		–
$(B + B)_I'$	$c,t + c,t$	2.904	−71.242	−9.01		–
$(B + C)_I$	$c,t + t,c$	2.919	−81.155	−8.13		–
$(B + C)_I'$	$c,t + t,c$	2.912	−81.008	−7.98		–
$(C + A)_I$	$t,c + c,c$	2.923	−91.185	−7.19	3.5	0.33
$(C + A)_I'$	$t,c + c,c$	2.924	−91.839	−7.85	10.5	0.99
$(C + B)_I$	$t,c + c,t$	3.061	−82.7563	−9.73		–
$(C + B)_I'$	$t,c + c,t$	2.920	−81.303	−8.28		–
$(C + C)_I$	$t,c + t,c$	2.929	−90.812	−6.99	1.9	0.18
$(C + C)_I'$	$t,c + t,c$	2.920[c]	−94.573	−10.76	1000	94.50

[a] The energy of Model γ with conformation A, B and C are −42.08, −31.11 and −41.91 cal mol^{-1}, respectively.

[b] The probability less than 0.01% not listed.

[c] Dimmer.

Table 3
Energy and probability of 9H-bonds configurations in Type II

Type	Conformation	H-bond length (Å)	E_{Total} (kcal mol^{-1})	ΔE_h (kcal mol^{-1})	σ (10^{-3})	Probability (%)
$(A + A)_{II}'$	$c,c + c,c$	2.931[a]	−89.569	−5.40	0.24	0.02
$(A + C)_{II}$	$c,c + t,c$	2.956	−88.696	−4.70	0.06	–
$(A + C)_{II}'$	$c,c + t,c$	2.958	−88.455	−4.46	0.04	–
$(B + A)_{II}$	$c,t + c,c$	2.908	−78.6897	−5.49		–
$(B + A)_{II}'$	$c,t + c,c$	2.908	−78.6897	−5.49		–
$(B + C)_{II}$	$c,t + t,c$	2.995	−78.2689	−5.24		–
$(B + C)_{II}'$	$c,t + t,c$	2.995	−78.2689	−5.24		–
$(C + A)_{II}'$	$t,c + c,c$	2.933[a]	−91.9580	−7.96	12.8	1.21
$(C + C)_{II}$	$t,c + t,c$	2.978	−88.761	−4.94	0.06	–

[a] Dimer.

Table 4
Energy and probability of 3H-bonds configurations in type III

Type	Conformation	H-bond length (Å)	E_{Total} (kcal mol^{-1})	ΔE_h (kcal mol^{-1})	σ (10^{-3})	Probability (%)
$(A + A)_{III}$	$c,c + c,c$	3.123	−88.791	−4.63	0.065	–
$(B + C)_{III}$	$c,t + t,c$	3.176	−81.372	−8.34[a]	0.0000003	$<3 \times 10^{-8}$
$(C + C)_{III}$	$t,c + t,c$	3.171	−89.4034	−5.58	0.181	0.02

[a] Including another NH···O=CH-bond.

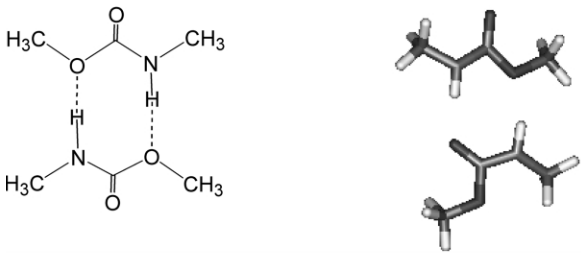


Fig. 6. H-bonded dimer between NH and alkoxyl oxygen.

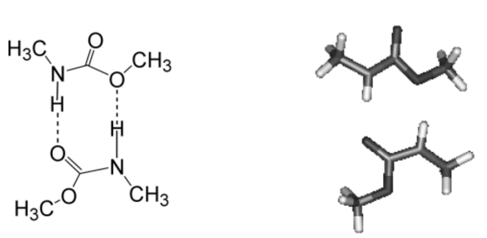


Fig. 7. H-bond dimer between NH and C=O, alkoxyl.

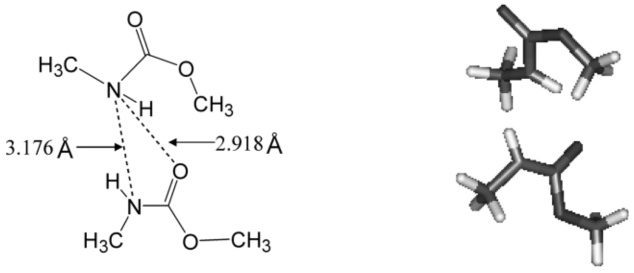


Fig. 8. Possible two H-bonds in B + C complex.

Model β and a Model γ molecule, we therefore cannot compare the probability of the H-bonds in the two systems by using the same zero point energy. We analyzed the second system separately. Table 5 shows that in the second system their H-bond lengths are obviously less than any other H-bond in the first system. One can also found that two of the three configurations (A + ether and C + ether), possessing almost the same lowest energies, almost evenly share the population of the H-bond in the second system, and the configuration of B + ether can be ignored as having ~10 kcal mol^{-1} higher energy.

3.3. The overview of the four types of H-bonds in polyether based polyurethane

The H-bond in polyether based polyurethane has been a comprehensive object in literature. In terms of structural features of the polymer, four types of H-bonds shown in Fig. 1 were early speculated. As mentioned above, most investigations were concentrated on Type I and Type IV. Actually, it is difficult to recognize H-bonding structures of Type II or Type III from experimental observations, such as infrared and Raman spectroscopy. In the preceding section, we found that based on the H-bond configuration energy Type I is the most stable H-bond pattern among the first three types, while Type II is unstable with an existent probability of 1–2% and Type III nearly absent. On the other hand, Type IV is the only H-bond pattern between the hard segment and the soft segment. Because we systemically studied all possible H-bond configurations, including various conformations of the urethane group and the pair conformations in the present work, we have a chance to evaluate the bond length and the bond strength of each of the four type H-bonds. Please note that the H-bond strength here equals to ΔE_h/bond.

Table 6 lists the average H-bond strength and average H-bond length of the four types of H-bonds. In order to obtain the H-bond parameters, we adopted different way to make the averages. According to H-bond configuration energy, the averages were calculated separately in each of the four types with their own zero point energies. The average is for a H-bond, possessing certain energy and certain length regarding O···O or O···N or N···N.

Table 5
Energy of 3H-bonds configurations in type IV

Type	H-bond length (Å)	E_{Total} (kcal mol^{-1})	ΔE_h (kcal mol^{-1})
(A + ether)$_{IV}$	2.884	−44.7519	−5.41
(B + ether)$_{IV}$	2.873	−34.3549	−5.98
(C + ether)$_{IV}$	2.895	−44.8775	−5.71

Structurally, the statistical calculation shows that Type IV has the shortest H-bond length 2.890 Å, and Type I 2.920 Å and Type II 2.933 Å, and that Type III has a somewhat larger bond length 3.159. Generally, the length of H-bond is less than 3.0 Å [23]. Type III is formed through a donor atom N and an acceptor atom N, while the van der Waals radius between the two atoms is 3.662 Å [23], which is obviously larger than formed Type III bond length. This manifests that Type III is still a weaker H-bond.

Energetically, obtained H-bond energy over number of bonds stands for the strength of the H-bond. The strongest H-bond here is of Type IV, −5.576 kcal mol^{-1}. Then the second one is of Type I, −5.430 kcal mol^{-1}, the third one is of Type III, −5.328 kcal mol^{-1}, and the last one of Type II, −4.023 kcal mol^{-1}. One may notice that in the early study the H-bond strength of Type I is larger than that of Type IV [13] (on the basis of 6.31G) in Table 1. However, in the early study the H-bond strength is not obtained from a reasonable conformational assemble average. If insularly studying on the two configurations as well as used there, MM can also give the same result (as shown in Table 1). The H-bond strength of Type IV being larger than that of Type I is consistent with the observation of vibrational spectroscopy [4,6,18].

Table 6 also shows that the H-bond of Type III is not so weak, even its existent probability is about 0.01% due to higher conformational energy. In the energy optimization, we noted that NH from one molecule would always be likely to form the H-bond with the C=O group from another molecule, although NH group was always put in the proper position with the other NH group for forming Type III H-bond before optimization. This result suggests that such a potentially possible H-bond is strongly competed by its neighbor C=O and affected by the steric volume from the two CH_3 in the urethane.

4. Conclusion

MM with COMPASS force filed was good in simulation of the H-bond interaction for polyurethane model molecules. Four types H-bond patterns usually speculated were systematically examined by searching all possible conformations of the donors and the acceptors in the system. A predominant interaction configuration, which consists of the two H-bonds belonging to Type I (NH···O=C), has been found among the 54 different H-bonded configurations in the hard segment interactions, while the two interactions of Type IV (NH···ether oxygen) are available among the three

Table 6
Average H-bond energy and H-bond length of the four types in polyether polyurethane

H-bond type	Type I (NH···C=O)	Type II (NH···OCO)	Type III (NH···NH)	Type IV (NH···OC)
Average H-bond length (Å)	2.920	2.933	3.159	2.890
H-bond energy[a] (kcal mol^{-1})	−5.430	−4.023	−5.328	−5.576

[a] This is for individual H-bond, if the interaction is through two H-bonds, the ΔE_h is just divided into two.

H-bonded configurations in the hard-soft segment interaction. NH is able to form the H-bond with alkoxyl O (Type II) in the special configuration but the probability is little, whereas NH hardly forms the H-bond with another NH (Type III).

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