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A thoroughly theoretical investigation into complexes formed by interaction of dimethyl sulfoxide with two water molecules

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Abstract

A computational study of the stability and the cooperative effect of hydrogen bonds in the complexes of dimethyl sulfoxide and two water molecules was undertaken at the MP2/6-311++G(2d,2p) level of theory. The cooperative energies of obtained complexes are significantly negative, indicating that there is a large cooperativity between types of hydrogen bonds. The existence of the O–H···O hydrogen bond present at dimer of water increases the stability of O–H···O and C–H···O hydrogen bonds in the ternary complexes compared to relevant binary complexes. By vibrational and NBO analyses, it is found that the magnitude of stretching frequency red shift of O–H bonds in the O–H···O hydrogen bonds is enhanced, whereas the extent of stretching frequency blue shift of C–H bonds in the C–H···O hydrogen bonds is weakened when the cooperativity of hydrogen bonds happens in the ternary complexes. Obtained results of AIM analysis and stabilization energies indicate the larger contribution of the O–H···O relative to the C–H···O hydrogen bond to cooperativity.

Keywords. Dimethyl sulfoxide, hydrogen bond, cooperativity.

1. INTRODUCTION

Noncovalent bonding interactions play an important role in crystal packing, molecular recognition, biological processes, and reaction selectivity [1, 2]. Understanding these interactions is thus essential for unraveling the mysteries of cellular function in health and disease as well as developing new drugs and materials that serve human life [3]. Among them, the subject of hydrogen bond A–H···B can be considered as a major interest due to a very important role in many fields of chemistry, physics, and biology. For instance, the presence of C–H···O/N hydrogen bonds has been found in protein, DNA double helix, RNA, [4]... However, the origin of the blue-shifting hydrogen bond has not been conformably understood [5, 6].

It is becoming increasingly apparent that cooperativity involving many molecules is an important component of intermolecular interactions, particularly those involving hydrogen bonds. When noncovalent binding interactions occur with positive cooperativity, the observed binding energy is greater than that in the isolated interaction, and vice versa that is negative cooperativity. The cooperativity of hydrogen bond plays an important role in controlling and regulating the processes occurring in living organisms. The occurrence of the cooperativity

among the subunits in hydrogen bonding system is accompanied with changes in the dynamics of the structures, for example, in DNA duplexes [7]. The cooperativity is also important in the formation of non-covalently bound aggregates of synthetic materials [8]. Therefore, the cooperativity of hydrogen bonds has paid much attention to theoretical and experimental researches.

The aqueous solutions of dimethyl sulfoxide (DMSO) have been extensively studied for their unique biological and physicochemical properties [9]. The use of the mixture of DMSO and CO₂ in PCA (Precipitation with a Compressed Antisolvent) process to precipitate proteins and polar polymers confronts some difficulties in both operation regions that are below and upper the critical pressure of the DMSO-CO₂ mixture. Some experimental studies suggested the use of water (H₂O) as a cosolvent of DMSO to modify the phase behavior of DMSO-CO₂ and solve limitations of the PCA process [10, 11]. Kirchner and Reiher [12] classified interactions between DMSO and water into O–H···O red-shifting and C–H···O blue-shifting hydrogen bonded contacts. The cooperativity between conventional and unconventional hydrogen bonds in DMSO aqueous solutions was reported by Li et al. [13, 14] with some of different structures. Consequently, the complexes between DMSO and two water molecules

are investigated thoroughly in the present work in order to consider the cooperative effect of interactions on the stability of complexes. Additionally, stretching vibrational frequency and natural bond orbital (NBO) analyses for the complexes and relevant monomers are also performed to understand further origin and cooperativity of interactions formed in complexes.

2. COMPUTATIONAL DETAILS

Geometry optimizations, harmonic vibrational frequencies of both monomers and complexes are carried out at the MP2/6-311++G(2d,2p) level of theory. Single point energy and basis set superposition errors (BSSE) are also calculated at the same level of theory. The interaction and cooperative energies are corrected both ZPE (zero point energy) and BSSE. All of the quantum chemical calculations mentioned above are executed using the Gaussian 09 program package [15]. The “atoms-in-molecules” (AIM) [16] analysis at the MP2/6-311++G(2d,2p) level is applied to determine the bond critical points (BCP) and to estimate electron densities and their Laplacians. Individual energy of each hydrogen bond (E_{HB}) is based on the formula of Espinosa-Molins-Lecomte: $E_{\text{HB}} = 0.5V(r)$, in which $V(r)$ is electron potential energy density at BCP [17]. Electron density in antibonding orbitals and electron density transfer between monomers originated from complexation are

calculated by means of the natural bond orbital (NBO) method using NBO 5.G software [18].

3. RESULTS AND DISCUSSION

3.1. Structures and AIM analysis

The geometric shapes and intermolecular distances of the complexes optimized at the MP2/6-311++G(2d,2p) level are displayed in Fig. 1, while the features of BCPs and individual energy of each hydrogen bond in the binary and ternary complexes are tabulated in table 1. Each complex is stabilized by different intermolecular contacts including C5–H6...O11 and O11–H12...O10 in **P1-B**; C1–H3...O11, C5–H7...O11 and O11–H12...O10 in **P2-B**; C1–H4...O11, C5–H8...O11 and S9...O11 in **P3-B**; C1–H2...O11, O14–H15...O10 and O11–H12...O14 in **P1-T**; C1–H3...O11, C5–H7...O11, O14–H15...O10 and O11–H12...O14 in **P2-T**; C1–H4...O11, C5–H8...O11, O14–H15...S9 and O11–H12...O14 in **P3-T**. There is a difference in structure between binary and ternary systems for the complexes of DMSO and H₂O that is presence of O–H...O interaction in H₂O...H₂O in the ternary complexes, except for **P3-T** with existence of O14–H15...S9 interaction as compared to S9...O11 interaction in **P3-B**. The complexes of ternary system found in present work were not reported by Li et al. [13, 14].

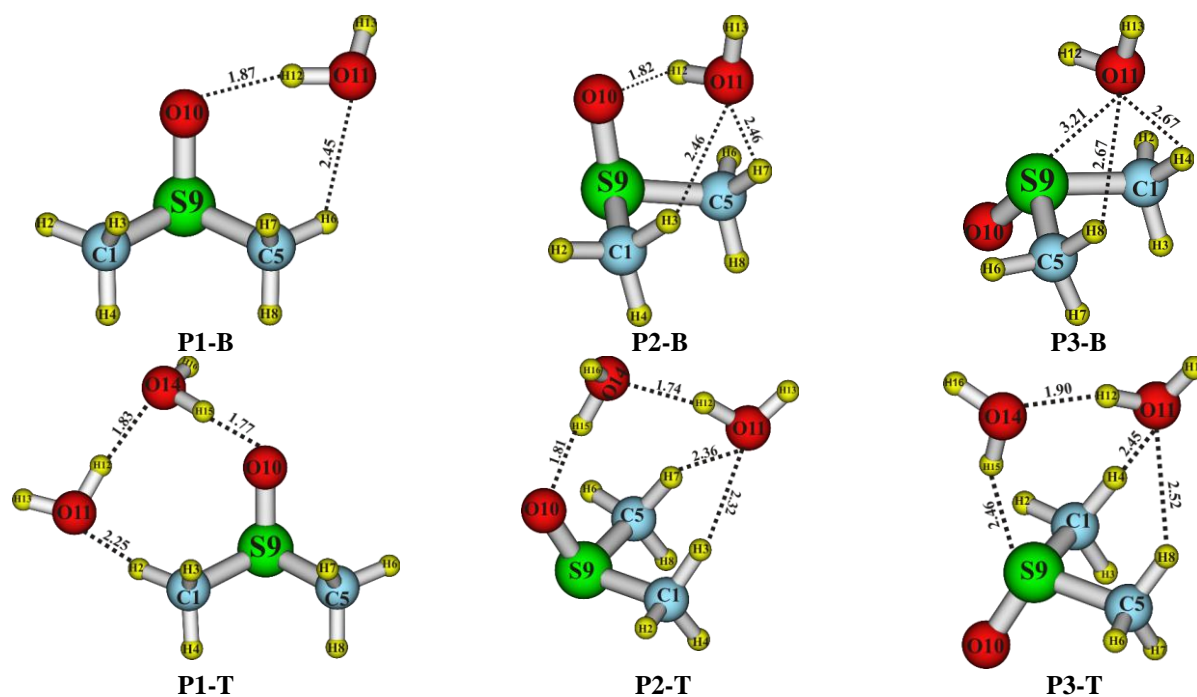


Figure 1: Stable geometries of complexes formed by interactions of DMSO with 1H₂O and 2H₂O at MP2/6-311++G(2d,2p)

Table 1: Selected parameters at the BCPs of intermolecular contacts at MP2/6-311++G(2d,2p)

Complex	Contacts	$\rho(r)$ (au)	$\nabla^2\rho(r)$ (au)	$H(r)^a$ (au)	E_{HB}^b (kJ.mol ⁻¹)
P1-B	C5-H6...O11	0.009	0.036	0.0013	-8.3
	O11-H12...O10	0.029	0.098	0.0000	-32.2
P2-B	C1-H3...O11	0.009	0.034	0.0011	-8.2
	C5-H7...O11	0.009	0.034	0.0011	-8.2
	O11-H12...O10	0.033	0.105	-0.0012	-37.5
P3-B	C1-H4...O11	0.007	0.023	0.0008	-5.6
	C5-H8...O11	0.007	0.023	0.0008	-5.6
	S9...O11	0.008	0.030	0.0009	-
P1-T	C1-H2...O11	0.014	0.048	0.0013	-12.4
	O14-H15...O10	0.035	0.112	-0.0015	-40.9
	O11-H12...O14	0.032	0.103	-0.0005	-35.2
P2-T	C1-H3...O11	0.011	0.041	0.0013	-10.1
	C5-H7...O11	0.011	0.038	0.0010	-9.8
	O14-H15...O10	0.038	0.117	-0.0022	-44.3
	O11-H12...O14	0.035	0.109	-0.0009	-38.0
P3-T	C1-H4...O11	0.009	0.032	0.0010	-8.0
	C5-H8...O11	0.009	0.029	0.0007	-7.4
	O14-H15...S9	0.018	0.044	0.0000	-14.6
	O11-H12...O14	0.026	0.092	0.0000	-28.3

^{a)}the total electron energy density; ^{b)}individual energy of each hydrogen bond.

All H...O(S) and S...O intermolecular distances are in the range of 1.74–2.67 and 3.21 Å respectively (table 1), which are shorter to sums of van der Waals radii of the relevant atoms (being 2.72 Å and 3.0 Å for H...O and H...S corresponding contact). This roughly suggests the presence of these intermolecular interactions in the complexes investigated. All the values of electron density ($\rho(r)$) and Laplacian ($\nabla^2\rho(r)$) at these BCPs are in the range of 0.007-0.035 au and 0.023-0.117 au, except for H15...O10 contact in **P2-T** has very large electron density of 0.038 au. All of them fall within the limitation criteria for the formation of hydrogen bond (0.002-0.035 au and 0.020-0.150 au for $\rho(r)$ and $\nabla^2\rho(r)$, respectively). Therefore, the intermolecular contacts in the complexes are considered as hydrogen bonds, except for S9...O11 chalcogen-chalcogen interaction in **P3-B**. The C-H...O and O-H...S interactions are weak hydrogen bonds as indicated by both the values $\nabla^2\rho(r) > 0$ and $H(r) \geq 0$, whereas very large values of $\rho(r)$ and negative values of $H(r)$ at BCPs of the O-H...O contacts are estimated, implying that these strong hydrogen bonds are partly covalent in nature. The formation of the S9...O11 chalcogen-chalcogen interaction in **P3-B** is more clarified by NBO analysis being discussed below.

As indicated in table 1, there is an increase in electron density at the BCPs and negative value of

E_{HB} in the order of C-H...O to O-H...S and to O-H...O, implying that the strength of hydrogen bonds tends to increase according to this trend. As a result, the role of the contribution of interactions formed into the total interaction energy of complexes decreases in going from O-H...O to O-H...S to C-H...O and S...O interaction. For both binary and ternary systems, a decrease of both electron density at the BCPs and the strength of O-H...O hydrogen bonds in the order of **P2** to **P1** to **P3** shape is observed. The obtained results suggest that the stability of complexes decreases in the order of **P2** to **P1** and finally to **P3** shape.

Compared with corresponding complexes in binary system, the electron densities at the BCPs in ternary complexes are larger, by 0.002-0.005 au for C-H...O and 0.005-0.006 au for O-H...O hydrogen bonds. Furthermore, the individual energies of the hydrogen bonds in ternary complexes are more negative than those in corresponding binary complexes by 1.6-4.1 kJ.mol⁻¹ for C-H...O hydrogen bonds and 6.8-8.7 kJ.mol⁻¹ for O-H...O hydrogen bonds. These results imply that the strength of hydrogen bonds is enhanced when cooperativity happens, and the larger magnitude of cooperativity is observed for the O-H...O hydrogen bond compared to C-H...O hydrogen bond. This result is different from publication reported by Li et al. [13], where the authors suggested the larger increase in

stability of the C–H⋯O relative to O–H⋯O hydrogen bond taken from the cooperativity. This should be due to the difference in the geometric structure of complexes investigated.

3.2. Interaction and cooperative energies

Interaction and cooperative energies of complexes at the MP2/6-311++G(2d,2p) level are summarized in Table 2. All interaction energies of the complexes for both binary and ternary systems are significantly negative, indicating that the obtained complexes are quite stable. Interaction energies for ternary complexes range from -30.3 to -52.7 kJ.mol⁻¹ with

ZPE + BSSE corrections, which is more negative than relevant binary complexes by *ca.* -24.4, -25.2 and -20.5 kJ.mol⁻¹ for **P1**, **P2** and **P3** shape respectively. As be seen in Table 2, the decreasing magnitude in complex strength is ordered in going from **P2** to **P1** and finally to **P3** shape for both binary and ternary systems, which is in good agreement with the results taken from the AIM analysis mentioned above. Thus, the **P2-T** complex is more stable than the **P1-T** and **P3-T** complexes by *ca.* 5.3 and 22.4 kJ.mol⁻¹ respectively. Remarkably, interaction energy of -27.5 kJ.mol⁻¹ for **P2-B** is rather close to that for DMSO⋯1H₂O complex (-28.3 kJ.mol⁻¹) reported by Li et al. [14].

Table 2: Interaction energy (ΔE , ΔE_{ABC}) and cooperativity energy (E_{coop}) of binary and ternary complexes at MP2/6-311++G(2d,2p), all in kJ.mol⁻¹

Complex	ΔE	Complex	ΔE_{ABC}	ΔE_{AB}	ΔE_{AC}	ΔE_{BC}	E_{coop}
P1-B	-29.6 (-23.0)	P1-T	-60.5 (-47.4)	-9.1 (-5.9)	-23.3 (-17.1)	-8.5 (-4.0)	-19.7 (-20.5)
P2-B	-35.3 (-27.5)	P2-T	-67.1 (-52.7)	-26.8 (-20.1)	-26.8 (-7.3)	-11.2 (-2.3)	-22.2 (-22.9)
P3-B	-13.6 (-9.8)	P3-T	-40.9 (-30.3)	-10.8 (-7.4)	-7.5 (-3.8)	-10.2 (-6.3)	-12.2 (-12.9)

Values in brackets for both ZPE and BSSE corrections, A = DMSO, B = H₂O, C = H₂O.

The interaction energy (-52.7 kJ.mol⁻¹) for the most stable complex of ternary system (**P2-T**) is more negative than that of DMSO⋯1H₂O (-28.28 kJ.mol⁻¹) and DMSO⋯2H₂O (-47.92 kJ.mol⁻¹) reported by Li et al. at the MP2/6-31++G(d,p) level [14]. However, the complex DMSO⋯3H₂O with interaction energy of -58.23 kJ.mol⁻¹ in the literature [14] is *ca.* 5.53 kJ.mol⁻¹ more stable than DMSO⋯2H₂O (**P2-T**) in the present work. These results show that the adding of water molecules into DMSO system leads to increase the stability of complexes.

The cooperative energy (E_{coop}) is applied here to evaluate the cooperativity of the hydrogen bonds in the ternary system. Cooperative energies are calculated using the expression:

$$E_{coop} = \Delta E_{ABC} - \Delta E_{AB} - \Delta E_{BC} - \Delta E_{AC}$$

Where ΔE_{AB} , ΔE_{BC} , ΔE_{AC} are the interaction energies of dimers A and B, B and C, A and C, respectively, in the optimized geometry of the ternary system. From Table 2, it can be seen that all the values of E_{coop} are significantly negative, indicating the hydrogen bonds in the ternary complexes work in concert with each other and enhance each other's strength. In these ternary systems, the absolute values of E_{coop} decrease in the order of **P2-T** > **P1-T** > **P3-T**, which is consistent with the increase of the interaction energy in this direction. It indicates that there is a good correlation between cooperativity and interaction energies of complexes examined. The

calculated energies due to cooperativity in the ternary complexes are from -12.9 to -22.9 kJ.mol⁻¹ with ZPE + BSSE corrections, which are significantly different with the values of -1.16 and -1.67 kJ.mol⁻¹ for two other structures of DMSO⋯2H₂O reported by Li et al. [14]. As a result, it should be noteworthy that the second O–H⋯O hydrogen bond between two water molecules in the ternary complexes found in our research induces such a significant change of cooperativity.

3.3. Vibrational and NBO analyses

To classify and gain a clearer view on the origin and cooperativity of the hydrogen bonds, the changes in the C(O)–H bond lengths and its stretching frequency, directions of electron density transfer (EDT) and the factors causing the red and blue shift of the C(O)–H bonds in hydrogen bonds at the MP2/6-311++G(2d,2p) level are given in table 3.

Following complexation, the C–H bond lengths are shortened by 0.0014–0.0036 Å and accompanied by a stretching frequency increase of 8.4-40.7 cm⁻¹, whereas an elongation of O–H bond lengths by 0.0084-0.0223 Å and a decrease in its corresponding stretching frequency from 167.1 to 438.4 cm⁻¹ are observed as compared to those in the relevant monomers. These results indicate that the C–H⋯O hydrogen bonds in the complexes belong to the blue-shifting hydrogen bond, while the O–H⋯O(S)

hydrogen bonds are red-shifting hydrogen bond. As shown in Table 3, an elongation of O–H bond lengths and a concomitant red shift of its stretching frequency increase in the order of **P3** < **P1** < **P2** for both binary and ternary systems, which is consistent with the increase in the stability of complexes mentioned above.

In going from binary complexes to corresponding ternary complexes, it is remarkable that there is an opposite change in the red and blue shift of O–H and C–H bonds in O(C)–H...O hydrogen bonds. Thus, a much larger red shift by *ca.* 90.8–120.7 cm⁻¹ of the stretching frequencies of

O–H bonds in the O–H...O hydrogen bonds is obtained, whereas a magnitude of stretching frequency blue shift of the C–H bonds in the C–H...O hydrogen bonds decreases by *ca.* 0.7–21.3 cm⁻¹ in the ternary complexes compared to the corresponding binary complexes. As a result, the cooperativity between types of hydrogen bonds induces an enhancement of magnitude of stretching frequency red shift of the O–H bonds in the O–H...O hydrogen bonds, but that causes a decrease in the magnitude of blue shift of the C–H bonds in the C–H...O hydrogen bonds.

Table 3: Changes of bond length (Δr) and corresponding stretching frequency ($\Delta \nu$) of C(O)–H bonds involved in hydrogen bond along with selected results for NBO analysis at MP2/6-311++G(2d,2p)

Complex	EDT	Hydrogen bond	Δr (Å)	$\Delta \nu$ (cm ⁻¹)	E_{inter} (kJ.mol ⁻¹)	q(C/O) (e)	q(H) (e)	$\Delta \sigma^*$ (C(O)–H) (e)	$\Delta \%s$ (C(O)) (%)
P1-B	0.021 ^{a)}	C5–H6...O11	-0.0028	29.7	2.9	-0.749	0.245	0.0004	0.77
	-0.021 ^{b)}	O11–H12...O10	0.0132	-261.5	50.0	-0.963	0.485	0.0208	3.16
P2-B	0.026 ^{a)}	C1–H3...O11	-0.0033	33.9	3.8	-0.760	0.238	-0.0006	0.94
	-0.026 ^{b)}	C5–H7...O11	-0.0033	34.3	3.8	-0.760	0.238	-0.0006	0.94
		O11–H12...O10	0.0172	-347.6	60.5	-0.971	0.485	0.0284	3.52
P3-B	0.006 ^{a)}	C1–H4...O11	-0.0036	38.7	1.3	-0.759	0.223	-0.0006	0.47
	-0.006 ^{b)}	C5–H8...O11	-0.0036	40.7	1.3	-0.759	0.223	-0.0006	0.47
		S9...O11	-	-	2.3/0.3	-	-	-	-
P1-T	0.025 ^{a)}	C1–H2...O11	-0.0014	8.4	14.2	-0.764	0.261	0.0048	1.52
	-0.019 ^{b)}	O14–H15...O10	0.0196	-382.2	78.7	-0.970	0.493	0.0292	4.19
		-0.006 ^{c)}	O11–H12...O14	0.0152	-300.3	57.7	-0.968	0.499	0.0239
P2-T	0.025 ^{a)}	C1–H3...O11	-0.0032	33.2	9.5	-0.762	0.245	0.0010	1.44
	-0.007 ^{b)}	C5–H7...O11	-0.0031	30.5	8.3	-0.762	0.245	0.0015	1.39
		-0.018 ^{c)}	O14–H15...O10	0.0223	-438.4	106.9	-0.972	0.499	0.0337
	O11–H12...O14	0.0168	-331.9	63.1	-0.974	0.495	0.0263	3.93	
P3-T	0.026 ^{a)}	C1–H4...O11	-0.0030	32.9	5.3	-0.763	0.237	0.0003	0.88
	-0.012 ^{b)}	C5–H8...O11	-0.0029	32.8	4.4	-0.762	0.236	0.0004	0.79
		-0.014 ^{c)}	O14–H15...S9	0.0084	-167.1	21.8	-0.950	0.466	0.0153
	O11–H12...O14	0.0107	-206.6	36.3	-0.964	0.490	0.0223	3.01	

^{a),b),c)} for charge of A, B, C respectively.

There are various trends of electron density transfer between DMSO and H₂O as a result of complex formation. The positive values of EDT(a) ranging from 0.006 to 0.026 e indicate that the electron density is transferred from DMSO to H₂O. The formation of S9...O11 chalcogen-chalcogen interaction in **P3-B** complex is resulted from electron density transfer of both from S9 lone pairs to $\sigma^*(\text{O11–H12}(13))$ orbital (2.3 kJ.mol⁻¹) and from O11 lone pairs to $\sigma^*(\text{S9–O10})$ orbital (0.3 kJ.mol⁻¹).

As shown in table 3, there are increases in s-character of the O(H) atoms from 2.17 to 4.32% and electronic population of the $\sigma^*(\text{O–H})$ orbitals

between 0.0153 and 0.0337 e for all complexes, meaning that an elongation of the O–H bond lengths and a red shift of its stretching frequency arise from an increase in electron population in the $\sigma^*(\text{O–H})$ orbitals overcoming an increase in s-character of the O(H) hybrid orbital. Remarkably, the increase in electron population of $\sigma^*(\text{O–H})$ orbitals is larger for ternary complexes than for binary complexes. For the C–H...O hydrogen bonds of binary complexes, a C–H bond contraction of and a blue shift of its stretching frequency in the C–H...O hydrogen bonds are contributed by a decrease of population in the $\sigma^*(\text{C–H})$ orbital and an increase of s-character

percentage of C(H) orbital, except for C5–H6···O11 hydrogen bond of **P1-B** complex. However, a C–H bond contraction accompanied by its stretching frequency blue shift in the C–H···O hydrogen bonds for all ternary complexes is mainly determined by an increase of s-character percentage of C(H) atoms since the population of the $\sigma^*(\text{C–H})$ orbital is enhanced upon complexation (*cf.* table 3). These results also support for observation of change in the magnitude of stretching frequency red and blue shift of the O(C)–H bonds in hydrogen bonds that there is cooperativity mentioned above.

From the structure of binary to corresponding ternary complexes, the $E_{\text{inter}}(n(\text{O}) \rightarrow \sigma^*(\text{O–H}))$ values are increased by *ca.* 28.2–46.4 kJ.mol⁻¹, while the $E_{\text{inter}}(n(\text{O}) \rightarrow \sigma^*(\text{C–H}))$ values are also increased by *ca.* 3.1–11.3 kJ.mol⁻¹. This suggests the contribution from the orbital interaction to the cooperativity is much larger for O–H···O as compared to C–H···O hydrogen bond, which is in good accordance with AIM analysis mentioned above. Furthermore, there is an increase in both negative charge on the O/C atoms and positive charge on H atoms in ternary complexes compared to binary complexes, making it easier than to form C(O)–H···O hydrogen bonds in ternary complexes. These results affirm again that the strength of C(O)–H···O hydrogen bonds is enhanced in ternary with respect to binary complexes.

4. CONCLUDING REMARKS

Interaction of dimethyl sulfoxide with two water molecules induces three quite stable complexes with interaction energies between -30.3 and -52.7 kJ.mol⁻¹ at MP2/6-311++G(2d,2p) level. The stability of obtained complexes is mainly determined by the O–H···O hydrogen bonds along with the complementary role of O–H···S and C–H···O hydrogen bonds. Obtained results show that there is a great cooperativity between both types of hydrogen bonds with cooperative energies from -12.9 to -22.9 kJ.mol⁻¹. In ring structure of DMSO···2H₂O, the formation of O–H···O hydrogen bond in the H₂O···H₂O dimer enhances the stability of O–H···O and C–H···O hydrogen bonds in the ternary complexes. The strength increase of the O–H···O hydrogen bonds is larger than that of the C–H···O hydrogen bonds when the cooperativity between types of hydrogen bonds happens. The water molecule plays a different role in two types of hydrogen bonds: proton-donor in O–H···O(S) red-shifting hydrogen bond and proton-acceptor in blue-shifting C–H···O hydrogen bond. In going from binary complexes to relevant ternary complexes, the

magnitude of stretching frequency red shift of the O–H bonds in the O–H···O hydrogen bonds is enhanced, while the magnitude of stretching frequency blue shift of C–H bonds in C–H···O hydrogen bonds is weakened.

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