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Influence of magnetic field on physical–chemical properties of the liquid water: Insights from experimental and theoretical models

Evelyn J.L. Toledo, Teodorico C. Ramalho, Zuy M. Magriotis *

Departamento de Química, Universidade Federal de Lavras, Campus Universitário, C.P. 3037, 37200-000 Lavras-MG, Brazil

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Abstract

This article examines the effect of a static magnetic field on liquid water. Experimental measure of viscosity, enthalpies and surface tension of water submitted to a magnetic field suggests that intra cluster hydrogen bonds were broken. From our theoretical and experimental data, we may conclude that the competition between the different hydrogen bonds networks (intra- and intermolecular) gives rise to the weakening of the hydrogen bonds intra cluster forming smaller cluster with stronger inter cluster hydrogen bonds.

Keywords: Magnetic field; Water; Clusters; Theoretical calculations

1. Introduction

Water presence is fundamental for the all life on the planet, because it is nutrient source and the place where chemical reactions happen. Thus, it is necessary to know its structure and geometry to understand its properties, but it is not easy. Several studies have been done in the attempt to understand it [1–13], but a lot of possibilities still exist to be explored.

In 1953, Vermeirem patented a technique that pointed to the possibility of making changes in water [14]. This technique consists of exposing water to a magnetic field. The changes in the structure of water when exposed a magnetic field are important in various applications. For instance, it has been reported that water gives rise to many phenomena when it is magnetized such as the increase in the compressive strength of concrete and in the precipitation process of calcium carbonate and [15,16], reduction of the corrosion rate of steel [17]. The change of various physical properties of water in applied magnetic fields has been reported too [18,19]. An increase of water viscosity under the influence of magnetic field has been explained on the basis of stronger hydrogen bonds [18]. An enhancement of water vaporization rate due to a magnetic field has been observed [19].

It is well-known that the water is formed of clusters and the more stable cluster numbers are called magic numbers. The sequence of magic numbers carries essential information about the electronic and ionic structure of the cluster and consequently the water properties. If it is possible modify the magic numbers, we can find many new alternative uses of water, because the importance of the other magic numbers is related to intrinsic proprieties of water. Thus, a lot of work has been devoted to identify the magic clusters of water (clusters: 1, 4, 6, 7, 11 and 13). The problem of the magic clusters is closely linked to the problem of searching for the global minimum potential energy of the clusters. The changes in the structure of water under the effect of an external magnetic field have been related and studies have found that various aspects of water structure changes when exposed to a magnetic field [20–24]. These changes were associated to hydrogen bonds [23].

Water treatment by magnetic field is still a controversial subject, because the reported results have low reproducibility and little consistence. In the treatment there are many factors difficult to control, such as magnetic impurities

* Corresponding author. Tel./fax: +55 35 3829 1889.
E-mail addresses: teo@ufla.br (T.C. Ramalho), zuy@ufla.br (Z.M. Magriotis).

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and quantity of dissolved oxygen, thus the experiments have been qualitative. An important way of outlining these problems is through theoretical calculations. They make it possible to foresee situations controlling many variables. The computational developments lead to theoretical calculations more accurate and faster.

In spite of the possibilities offered by computational resources, few theoretical works are devoted to the magnetic treatment of water. Changes in the internal energy and heat capacity of pure water by an external magnetic field were investigated using Monte Carlo simulations [21]. The decrease of the self-diffusion coefficient of the water molecules was also studied by molecular dynamics simulation [20]. Theses changes were correlated with the weakness of the van der Waals bonds between water molecules [25], and the weakness and enhancing of the hydrogen bonds [20–22,24]. So it would seem like it is possible to obtain new clusters arrangements and then stabilize them to create news magic numbers.

In this study, the influence of a magnetic field in the energy of the clusters and on the interactions of the water molecules using theoretical calculations and the alterations on the physical-chemical properties, through experimental measures of vaporization enthalpy, viscosity and surface tension were investigated.

2. Experimental procedure

For the magnetic treatment a covered glass flask containing water was left on the north pole of a magnet for three hours. The magnet was a disc 18 mm thick, 150 mm in diameter with a hole of 64 mm in diameter. The intensities of the magnetic field at the extremities from the center were in the range of 45–65 mT. The schematic diagram of the experimental setup is in Fig. 1. All the magnetic treatments were accomplished to 295 K and 91.6 kPa.

The vaporization enthalpy was obtained by vapor pressure at several temperatures measurements [26]. The viscosity experiments were carried out in an Ostwald viscosimeter. The surface tension was calculated by the weight drop or volume drop method [27].

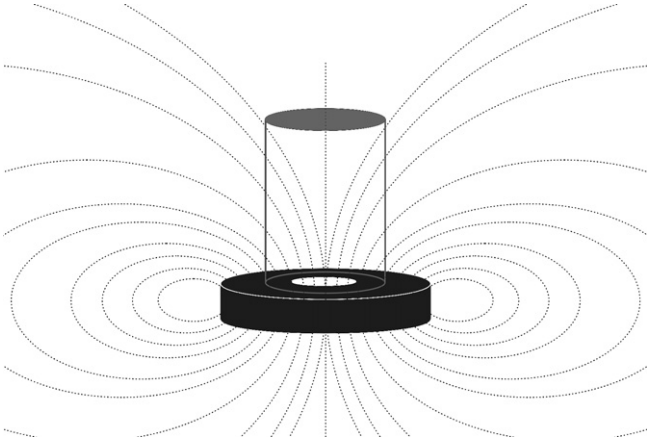

Fig. 1. Schematic diagram of the experimental setup.

All the experiments were accomplished to 295 K, 91.6 kPa and repeated 10 times. The results were statically verified by variance analysis and *T*-test.

3. Computational methodology

All properties were calculated at DFT (Density Functional Theory) level with the density functional Becke's three-parameter exchange functional and the gradient-corrected functional of Lee, Yang, and Paar (B3LYP) [28,29]. This functional has been shown to be particularly accurate in the calculation of molecular magnetic properties [30]. For all calculated properties, we considered the cc-pVDZ (polarized double-zeta) basis sets. The influence of the external apparent magnetic field on the ground state PES (potential energy surface) was studied using single-point energy calculations along with water cluster geometries obtained from the literature [31]. Several works have used the DFT approach to study hydrogen-bonded clusters [32–34]. The success of some of these investigations could be attributed to the fact that the DFT approach includes exchange correlation effects. The *ab initio* calculations in the present study were performed using GAUSSIAN98 program package [35]. The apparent magnetic field was simulated indirectly adding a finite electrical field. This strategy has also been used for other research groups [21,36,37]. Herein, we have used a well-known relation between atomic unity (a.u.) and the energy flux density [21,36,37].

It should keep in mind that we have studied the water clusters with same charge and structural facts in different conditions. In line with that, a qualitative behavior may be obtained on the influence of an apparent magnetic field on the system [2].

The apparent magnetic field was calculated considering constant the speed of the molecules. So the electric-field magnitude of 0.01 a.u. is equivalent to 17 T [36,38] and the intensities in the range from 0 to 14 T are normally employed in magnetized water studies [18–22,24,25,39]. Therefore, our calculations in this study, are performed in range from 0 to 34 T. The basis set superposition error (BSSE) for the complexation-induced results was estimated using the counterpoise correction method [39,40].

4. Results and discussion

Viscosity is an internal property of a fluid that offers resistance to flow. The flow rate of a liquid depends on the magnitude of the intermolecular forces and the shapes of the molecules, the larger the molecule the slower they move. The viscosity of a liquid can change appreciably with temperature. But temperature is not the only variable that has influence on viscosity; studies have found that the magnetic field also influences the viscosity [18,41].

Surface tension is caused by the attraction among the molecules of the liquid due to various intermolecular forces. This forms a surface film which makes it more difficult to move an object through the surface than to move it when it is completely submersed.

Enthalpy is a measure of heat in the system. The enthalpy of vaporization is the energy required to transform a given quantity of a substance into a gas. It can be viewed as the energy required to overcome the intermolecular interactions in the liquid.

Viscosity (η), surface tension (γ) and vaporization enthalpy (ΔH_{vap}) are properties that are correlated with the intermolecular forces. So changes in these properties can be related with changes in these forces. The values found for the enthalpy, viscosity and surface tension are in Table 1.

All measurements were carried out in the same temperature (295 K) and magnetic treatment conditions with intention of reducing the errors. The results were submitted to variance analysis and *T*-test for validation of the increase tendencies of the measured parameters. The statistic analyses showed that for a reliability of 95% the values of the parameters for the water in absence of magnetic field and for the water submitted to the magnetic treatment were different.

The results show that the viscosity increased when the water was submitted to the magnetic treatment. The same tendency was observed in the surface tension and in the enthalpy and they were reported in the literature [18,19]. Increase in these physical–chemical properties means an increase in the molecular interactions.

The hydrogen bonds can be inter- and intra cluster. The competition of the interactions inter- and intra clusters in the system $Fe_4(PO_4)_3(OH)_3$ has been reported in the literature [42]. However, discussions of these two interactions for water have not been found to date.

Supposing that the clusters are only present in the gaseous phase, during the vaporization process so much the interactions inter as well as the intra are broken. Therefore, the increase of the vaporization enthalpy can be caused so much by the increase in the interactions of hydrogen intra clusters as well as the inter clusters, so for this property it is not possible to separate the effects of the magnetic field in the two interactions.

Regarding viscosity and surface tension, the inter clusters interactions are more important than the intra. The increase of these properties can be related to the increase of the inter clusters interactions.

In view of that, we suggested that the magnetic field weakens the intra cluster hydrogen bonds, breaking the larger clusters, forming smaller clusters with stronger inter cluster hydrogen bonds. Zhou [21] using theoretical calculations, suggested that the application of a magnetic field favored the breaking of the connections of the clusters, obtaining, then, smaller clusters and with larger numbers of neighbors.

Agreeing with the experimental data, our theoretical calculations show that the magnetic field is capable of affecting some properties water. In view of the large number of possible geometries for the larger clusters, there would be several minima on a shallow potential-energy surface, and it becomes extremely difficult to locate the true energy minimum for each cluster. Thus, the coordinates of water clusters were taken from Maheshwary's work [31]. The energy of molecular interaction was calculated using Eq. (1).

$$\Delta E_b = [E(\text{cluster}) - nE(\text{monomer})]/n \quad (1)$$

where ΔE_b is the intra cluster binding energy for the water molecule of the cluster, n is the number of water molecules of the cluster and E(monomer) is the energy of the monomer in the same conditions as the clusters. The binding energy of the bulk system (intra and inter) was calculated using Eq. (2), as suggested by Lee [2].

$$\Delta E = A/n + B \quad (2)$$

Table 2 shows those values for the studied clusters. The results for ΔE and ΔE_b for $n \to \infty$ are in Tables 3 and 4, respectively. The constant B in Eq. (2) should correspond to the binding energy of the bulk system (intra and inter). This could be attributed to intra cluster binding energy, however the inter energy is very small compared with the intra. So in the sum of both the prevails intra, it can be considered that the term corresponds the energy intra molecular.

It is observed that, in the absence of magnetic field, the value of binding energy show a small deviation the experimental result, demonstrating that the theoretical methodology reproduced the experimental data in a reliable way. Calculations performed with the use of the methods described above show that often clusters of a higher symmetry group possess relatively low energy. Thus, the symmetric cluster configurations are often of particular interest. The process of searching the symmetric cluster

Table 1
Vaporization enthalpy, surface tension and viscosity

	ΔH_{vap} (kJ mol^{-1})	γ (mN m^{-1})	η (μPa s)
Water	50.86 ± 0.46	72.27 ± 0.37	964.42 ± 1.19
Magnetized water	68.86 ± 0.49	75.50 ± 0.23	996.63 ± 4.42
Theoretical [41]	44.12	72.27	961.10

Table 2
A and *B* values (Eq. (2))

Field (T)	*B* (kcal)	*A* (kcal)
0.00	−12.2931	18.59342
0.343	−12.3245	18.71892
0.688	−12.3308	18.8005
1.032	−12.3433	18.88835
1.37	−12.3496	18.9762
6.58	−12.497	20.338
11.68	−12.611	21.611
17.00	−12.7889	23.01743
34.00	−13.1082	26.88573

Table 3
Intra cluster binding energy for $n \to \infty$

Field (T)	ΔE (kcal/mol)
Experimental [2]	−11.30
0.00	−12.2931
0.343	−12.3245
0.688	−12.3308
1.032	−12.3433
1.37	−12.3496
6.58	−12.497
11.68	−12.611
17.00	−12.7889
34.00	−13.1082

configurations can be speed up significantly. Then, to make sure that our calculations are correct, we selected the clusters geometries cluster from previous papers [31] (see Fig. 2).

Table 3 shows also that the increase in magnitude of the field decrease the intra cluster binding energy, these results agree well with the other data from the literature [21].

When the magnetic field is applied, we observed an alteration in the intra clusters binding energy of the water clusters. For small magnetic fields (B), for instance $B = 0.343$ T, the alteration was about 100 cal, this result is in good agreeing with our experimental data. Thus, for the smaller external apparent magnetic fields a visible variation of the cluster stability was not observed. However, for higher magnitudes of apparent magnetic fields, for instance $B = 17$ T, a significant alteration of the intra cluster binding energy is observed. It should be kept in mind, however, that all water molecule clusters were sensitive to the magnetic field employed.

We had previously seen that $B = 17$ T caused a decrease in the interactions, very strong when compared to the other fields studied. Now we can see that $B = 17$ T reduced the stability of the clusters with $n = 2$, 7, 11, 14 and 15, and increased the stability of the clusters with $n = 5$, 6, 9, 10 and 13. The binding energy in Fig. 3 and Table 4 show that the clusters with 3, 4, 8 and 12 water molecules are relatively stable compared to other water clusters. The stable conformer of the water cluster tend to form maximum number of planar three–four member rings as already noted by Lee [2].

It is clear from Fig. 3 that the apparent magnetic field decreases the stability of each cluster. This means that the external field can cause a weakening of intra clusters H bonds and the diminishing of the average number hydrogen bonds between water molecules. This shows that the content of monomer water molecules and dimmer water molecules will go up if water is exposed to an apparent magnetic field. In other words, larger clusters are broken to form smaller clusters.

As mentioned by other authors [21] an external magnetic field can change water–water interaction and increase the distance between water molecules. However, in this paper, in order to make sure that the conclusions drawn from this simulation are correct for systems of different sizes, we kept the clusters arrangements constant in order to eliminate that structural effect. Thus our observations are just focused on the strength of the hydrogen chemical bonds. In line with this observation, a conclusion could be made that an external magnetic field can weaken hydrogen bonds or reduce the mean number of hydrogen bonds.

Turning now to experimental data, we may note that viscosity, surface tension and enthalpy increased when water was submitted to an external magnetic field. Thus, the magnetic field constrains the movement of the water molecules, and hence changes both the thermal conduction and the viscosity in the liquid state. In this sense, the magnetic field would induce a tighter bonds between the water molecules, increasing the inter clusters interactions. However, from our theoretical calculations, we observed a decrease in the intra cluster binding energy of the water molecules. Surprisingly, this conflicting result is also described in other works [21] and in spite of great importance, to our knowledge; it has not been explained so far. Nevertheless, based on our experimental and theoretical data, we could suggest that there is a competition between inter and intra cluster interaction. For instance, as noted by

Table 4
Intra cluster binding energy (kcal/mol)

	0.00 T	0.343 T	0.688 T	1.032 T	1.37 T	6.58 T	11.68 T	17.00 T	34.00 T
$(H_2O)_2$	−2.89552	−2.86028	−2.80175	−2.74322	−2.6847	−1.7806	−0.9338	−0.0036	2.8868
$(H_2O)_3$	−6.17103	−6.17395	−6.17338	−6.17283	−6.17228	−6.1662939	−6.1582	−6.1531	−6.15261
$(H_2O)_4$	−7.98339	−7.98797	−7.98814	−7.98833	−7.98853	−7.9944856	−7.9982	−8.0064	−8.04756
$(H_2O)_5$	−8.29284	−8.30064	−8.30243	−8.30423	−8.30604	−8.3344596	−8.3652	−8.4007	−8.53078
$(H_2O)_6$	−8.85282	−8.87201	−8.88385	−8.89571	−8.90759	−9.0954736	−9.2709	−9.4704	−10.1237
$(H_2O)_7$	−9.47237	−9.47760	−9.47116	−9.46473	−9.45831	−9.361286	−9.2679	−9.1682	−8.86513
$(H_2O)_8$	−10.4687	−10.4709	−10.4710	−10.4712	−10.4714	−10.473611	−10.474	−10.477	−10.4806
$(H_2O)_9$	−10.4375	−10.4458	−10.4479	−10.4500	−10.4521	−10.487602	−10.519	−10.557	−10.6904
$(H_2O)_{10}$	−10.6855	−10.6964	−10.6987	−10.7010	−10.7033	−10.741077	−10.773	−10.811	−10.9331
$(H_2O)_{11}$	−10.3896	−10.3859	−10.3799	−10.3738	−10.3678	−10.278343	−10.195	−10.109	−9.34098
$(H_2O)_{12}$	−11.1233	−11.1383	−11.1384	−11.1386	−11.1389	−11.1462	−11.153	−11.167	−10.3994
$(H_2O)_{13}$	−10.6362	−10.7910	−10.8002	−10.8094	−10.8186	−10.966006	−11.105	−11.2647	−11.8039
$(H_2O)_{14}$	−10.2226	−10.2079	−10.1912	−10.1746	−10.1579	−9.90249	−9.6619	−9.40076	−8.60326
$(H_2O)_{15}$	−11.3319	−11.3209	−11.3078	−11.2948	−11.2817	−11.083144	−10.897	−10.6974	−10.1033

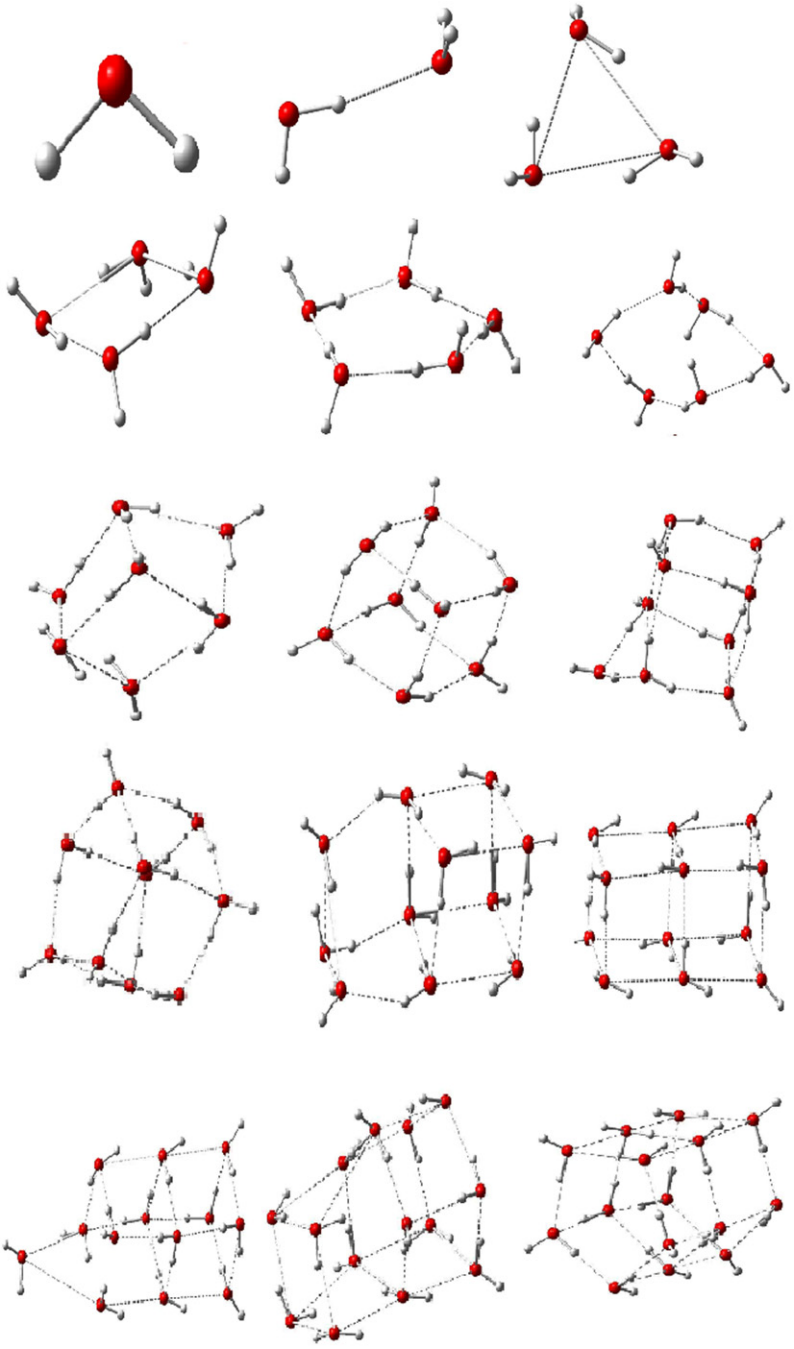

Fig. 2. Cluster geometries [31].

Zhou and co-workers using Monte Carlo simulation [21] whereas the magnetic field weakens the hydrogen bonds intra clusters, it was found that the second neighbor solvation shell is also strongly affected by the magnetic field, increasing the numbers of neighbors. This is the range which is very significant to the dielectric properties and reactivity of water.

Obviously, the reduction of heat capacity results from the reduction of the mean number of hydrogen bonds of the water system in an external magnetic field. It must be pointed out that the energy of the hydrogen bond is very sensitive to the distance between the bonds molecules. Formation or breaking of hydrogen bonds between the nearest molecules can increase or decrease. It demonstrates that the interaction of the magnetic moment can weaken or partially break hydrogen bonds in a water system and some water molecules may be separated from the water molecule cluster and become free monomer molecules. Because monomer water molecules can easily penetrate through biological cell walls, the water exposed to an external magnetic field can accelerate plant growth although the quantitative evaluation for the biological effect of a magnetic field

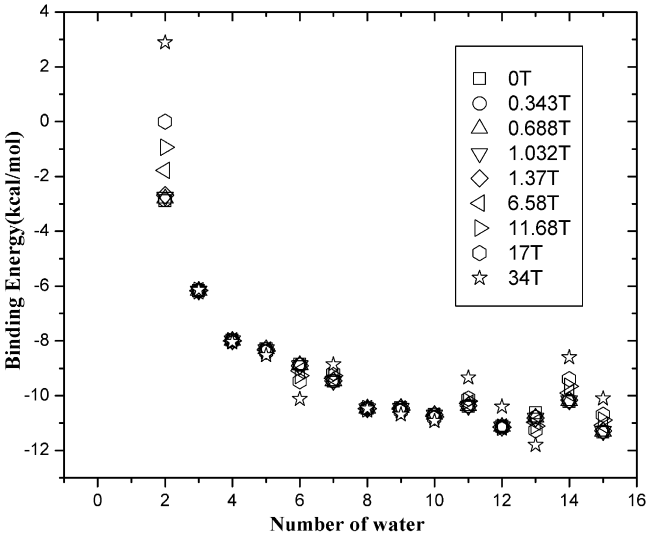

Fig. 3. Variation of energy with apparent magnetic field.

is difficult to obtain. This could be a reasonable explanation for the changing of various physicals properties of water in applied magnetic fields.

In light of this discussion, we suggest that the magnetic field weakens the hydrogen bonds intra clusters, breaking the larger clusters, forming smaller clusters. Magnetic fields break or distort the hydrogen-bond angle by causing a reorientation of the water molecules, and hence weaken or destroy the hydrogen-bond intra cluster network. However, it should be kept in mind that, the paramagnetic contribution from the magnetic susceptibility increases significantly due to breaking of the hydrogen bonds intra clusters. Weak interactions such as hydrogen bonds in H_2O are considered to contribute to the paramagnetic term. It is well known that the paramagnetic term of the magnetic susceptibility result in strengthening the hydrogen bonds [43–45]. In addition, when larger water clusters break forming smaller cluster, more stable water systems are formed by maximizing the number of the planar shaped four membered water rings [2] which is easier to occur with smaller clusters. So, we suggest that the magnetic field weakens the stronger intra clusters hydrogen bonds, breaking the larger clusters, forming smaller clusters with stronger inter cluster hydrogen bonds. Then, it would be feasible to obtain new clusters arrangements and then stabilize them to create new magic numbers.

5. Conclusion

This article has examined the effect of a static apparent magnetic field, which indirectly calculated on liquid water. It has been shown that an external magnetic field influences the number of hydrogen bonds, the structure of liquid water, and the self-diffusion coefficient of the water molecules external magnetic field. Through experimental measures of viscosity, enthalpies, surface tension of water submitted the magnetic field, it is suggested the hydrogen bonds hydrogen were broken which increased the force of the reminding bonds. Because DFT calculations are being used extensively for the study of van der Waals and hydrogen-bonded clusters [25] and B3LYP parameterization is often used, we have carried out DFT calculations with B3LYP parameterization using the cc-pvDZ. From our theoretical and experimental data, we may conclude that the competition between the different hydrogen bonds networks (intra- and intermolecular) gives rise to the weakening of the hydrogen bonds intra-cluster forming smaller cluster with stronger inter cluster hydrogen bonds.

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Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at doi:10.1016/j.molstruc.2008.01.010.

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