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Water Alignment Energy and Liquid-Liquid Critical Point

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Abstract: *The first 55 water alignment energies have been calculated and the equivalent in Kelvins of the 13th energy has been compared with the temperature of the liquid-liquid critical point (LLCP).*

Keywords: *Water alignment energy, temperature of the water liquid-liquid critical point (LLCP)*

1. Introduction

Let us calculate the first 55 water alignment energies and the equivalent in Kelvins of the 13th energy compare with the temperature of water liquid-liquid critical point (LLCP)[1].

2. The Alignment Energy

The alignment energy of the atom or molecule enables the alignment of the electron with its atom or molecule nature [2],[3],[4],[5],[6],[7],[8],[9]. Let us extend the concerned concept including the alignment of the electron with its cluster nature, too. An example of a water molecule cluster is presented in Figure 1.

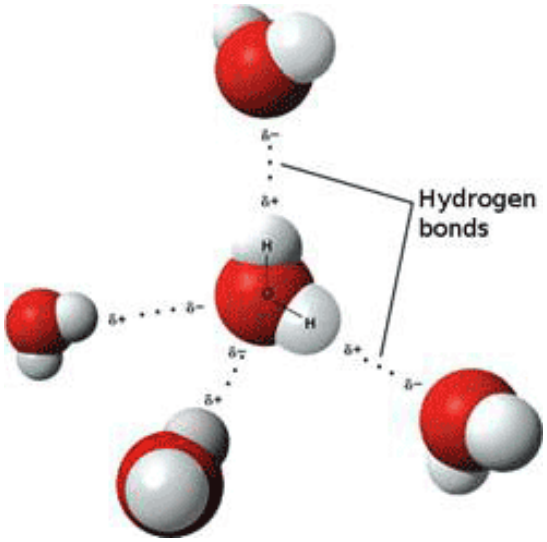

Figure1. *An example of water molecule cluster*

Also for water molecule clusters the next formula should be applicable:

$$Wk_{alignment} = \left(\frac{R_{unaligned}}{R_{aligned}} - 1\right) m_{electron}^{rest} c^2. \quad (1)$$

Where $R_{unaligned}$ in our present case is the unaligned modified ratio of water molecule cluster mass to electron mass:

$$R_{unaligned} = \frac{m_{cluster}}{m_{electron}^{rest}}\, s(1). \quad (2)$$

The factor *s(1) = 1,696 685 529…* is the average elliptic-hyperbolic manifestation of one (n = 1) elliptic Compton wavelength of the electron given by the next equation:

$$s(n) = n\left(2 - \frac{1}{\sqrt{1+\frac{\pi^2}{n^2}}}\right), n \in \mathbb{N}. \quad (3)$$

And the aligned modified ratio $R_{aligned}$ is given by the same equation(3) for the down rounded unaligned modified ratio ($n = ROUNDDOWN\ (R_{unaligned})$) as follows:

$$R_{aligned} = s\left(\text{ROUNDDOWN}\left(R_{unaligned}\right)\right). \quad (4)$$

3. THE WATER ALIGNMENT ENERGY

Using the data from the references[10],[11] and applying the equations(1),(2),(3),(4) the alignment energies of water molecule H_2O and its clusters $(H_2O)_n$, $1<n\leq55$ have been calculated. The alignment characteristics are presented in Table 1.

Table1. *The alignment characteristics of water molecule H_2O and its clusters $(H_2O)_n$, $1<n\leq55$*

Water	Mass (Da)	Unaligned R	Aligned R	Alignment energy (eV)	Alignment energy equivalent (K)
H_2O	18,010565	55704,309433	55704,000089	2,837763052	32930,87
$(H_2O)_2$	36,021130	111408,618866	111408,000044	2,838372562	32937,95
$(H_2O)_3$	54,031695	167112,928299	167112,000030	2,838485434	32939,26
$(H_2O)_4$	***72,042260***	***222817,237733***	***222817,000022***	***0,545155096***	***6326,26***
$(H_2O)_5$	90,052825	278521,547166	278521,000018	1,003845703	11649,15
$(H_2O)_6$	108,063390	334225,856599	334225,000015	1,309637641	15197,71
$(H_2O)_7$	***126,073955***	***389930,166032***	***389930,000013***	***0,21756672***	***2524,76***
$(H_2O)_8$	144,084520	445634,475465	445634,000011	0,54519319	6326,70
$(H_2O)_9$	162,095085	501338,784898	501338,000010	0,80001371	9283,77
$(H_2O)_{10}$	***180,105650***	***557043,094332***	***557043,000009***	***0,086526262***	***1004,10***
$(H_2O)_{11}$	198,116215	612747,403765	612747,000008	0,336712025	3907,38
$(H_2O)_{12}$	216,126780	668451,713198	668451,000007	0,545200244	6326,79
$(H_2O)_{13}$	***234,137345***	***724156,022631***	***724156,000007***	***0,015964807***	***185,26***
$(H_2O)_{14}$	252,147910	779860,332064	779860,000006	0,217579158	2524,90
$(H_2O)_{15}$	270,158475	835564,641497	835564,000006	0,392311685	4552,59
$(H_2O)_{16}$	288,169040	891268,950931	891268,000006	0,545202713	6326,81
$(H_2O)_{17}$	306,179605	946973,260364	946973,000005	0,140492887	1630,35
$(H_2O)_{18}$	324,190170	1002677,569797	1002677,000005	0,290385778	3369,79
$(H_2O)_{19}$	342,200735	1058381,879230	1058381,000005	0,424500531	4926,12
$(H_2O)_{20}$	360,211300	1114086,188663	1114086,000004	0,086532357	1004,17
$(H_2O)_{21}$	378,221865	1169790,498096	1169790,000004	0,217581462	2524,93
$(H_2O)_{22}$	396,232430	1225494,807530	1225494,000004	0,336717062	3907,44
$(H_2O)_{23}$	414,242995	1281199,116963	1281199,000004	0,046648413	541,33
$(H_2O)_{24}$	432,253560	1336903,426396	1336903,000004	0,162978171	1891,28
$(H_2O)_{25}$	450,264125	1392607,735829	1392607,000004	0,270001589	3133,24
$(H_2O)_{26}$	468,274690	1448312,045262	1448312,000003	0,015968414	185,31
$(H_2O)_{27}$	486,285255	1504016,354695	1504016,000003	0,120508913	1398,45
$(H_2O)_{28}$	504,295820	1559720,664129	1559720,000003	0,217582268	2524,94
$(H_2O)_{29}$	522,306385	1615424,973562	1615424,000003	0,30796094	3573,74
$(H_2O)_{30}$	540,316950	1671129,282995	1671129,000003	0,086533486	1004,18
$(H_2O)_{31}$	558,327515	1726833,592428	1726833,000003	0,175308608	2034,37

$(H_2O)_{32}$	576,338080	1782537,901861	1782537,000003	0,258535311	3000,18
$(H_2O)_{33}$	594,348645	1838242,211294	1838242,000003	0,058735397	681,60
$(H_2O)_{34}$	612,359210	1893946,520728	1893946,000003	0,140494996	1630,38
$(H_2O)_{35}$	630,369775	1949650,830161	1949650,000003	0,217582641	2524,94
$(H_2O)_{36}$	648,380340	2005355,139594	2005355,000002	0,035570313	412,78
$(H_2O)_{37}$	666,390905	2061059,449027	2061059,000002	0,111326828	1291,89
$(H_2O)_{38}$	684,401470	2116763,758460	2116763,000002	0,183096179	2124,74
$(H_2O)_{39}$	702,412035	2172468,067893	2172468,000002	0,015969082	185,31
$(H_2O)_{40}$	720,422600	2228172,377327	2228172,000002	0,086533881	1004,18
$(H_2O)_{41}$	738,433165	2283876,686760	2283876,000002	0,153656513	1783,11
$(H_2O)_{42}$	756,443730	2339580,996193	2339580,000002	0,217582844	2524,94
$(H_2O)_{43}$	774,454295	2395285,305626	2395285,000002	0,065200411	756,62
$(H_2O)_{44}$	792,464860	2450989,615059	2450989,000002	0,128231344	1488,06
$(H_2O)_{45}$	810,475425	2506693,924492	2506693,000002	0,188460916	2187,00
$(H_2O)_{46}$	828,485990	2562398,233926	2562398,000002	0,046649566	541,35
$(H_2O)_{47}$	846,496555	2618102,543359	2618102,000002	0,106051941	1230,68
$(H_2O)_{48}$	864,507120	2673806,852792	2673806,000002	0,162979229	1891,30
$(H_2O)_{49}$	882,517685	2729511,162225	2729511,000002	0,03037025	352,43
$(H_2O)_{50}$	900,528250	2785215,471658	2785215,000002	0,086534064	1004,19
$(H_2O)_{51}$	918,538815	2840919,781091	2840919,000002	0,140495387	1630,38
$(H_2O)_{52}$	936,549380	2896624,090525	2896624,000002	0,015969316	185,32
$(H_2O)_{53}$	954,559945	2952328,399958	2952328,000002	0,069225757	803,33
$(H_2O)_{54}$	972,570510	3008032,709391	3008032,000002	0,120509749	1398,46
$(H_2O)_{55}$	**990,581075**	**3063737,018824**	**3063737,000002**	**0,003139391**	**36,43**

We can see in Table 1 that the alignment energy $W_{alignment}^{(H_2O)_{13}} = 0{,}015964807$ eV of water molecule cluster $(H_2O)_{13}$ consisted of 13 molecules H_2O is the smallest amongst the first 54 alignment energies and could determine the liquid-liquid critical point (LLCP) of water. Indeed, such energy is available at temperature T=185,26 K which lies between the recently proposed values of 170 K and 190 K for the temperature of the liquid-liquid critical point (LLCP) of water[1]. Water cluster $(H_2O)_{13}$ can be regarded as the most stable tetrahedron-like cluster consisted of four connected tetrahedrons with three common vertices. We can also see in Table 1 that the stability of tetrahedrons having common vertices increases with the decreased alignment energy in the following order: the tetrahedron $(H_2O)_4$ itself is the least stable; two tetrahedrons with one common vertex $(H_2O)_7$ are more stable; three tetrahedrons with two common vertices $(H_2O)_{10}$ are still more stable; and finally four tetrahedrons with three common vertices $(H_2O)_{13}$ are the most stable. $(H_2O)_{13}$ clusters should represent the lighter phase of two liquids in the equilibrium.

4. Conclusion

It seems that the alignment energy of water cluster $(H_2O)_{13}$ determines the temperature of the water liquid-liquid critical point (LLCP) to be at T= 185 K.

Instead of Dedication

Figure1. *Save water and your health*

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