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Hydrogen Alignment Energy and Liquid-Liquid Critical Point

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Abstract: *The difference between the hydrogen molecule and hydrogen atom alignment energy has been calculated and its equivalent in Kelvins compared with the temperature of the Liquid-Liquid Critical Point (LLCP).*

Keywords: *hydrogen alignment energy, temperature of the Liquid-Liquid Critical Point (LLCP)*

1. Introduction

Let us calculate the difference between the hydrogen molecule and hydrogen atom alignment energy and compare its equivalent in Kelvins with the temperature of the Liquid-Liquid Critical Point (LLCP).

2. The Alignment Energy

The alignment energy of the atom or molecule enables the alignment of the electron with its atom or molecule nature [1], [2], [3], [4],[5],[6],[7]. It is given by the next formula:

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

Where $R_{unaligned}$ is the unaligned modified ratio of atom or molecule mass to electron mass:

$$R_{unaligned} = \frac{m_{atom\ or\ molecule}}{m_{electron}^{rest}} s(1). \tag{2}$$

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

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

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:

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

3. The Hydrogen Alignment Energy

Using the data from the reference [8], [9] and applying the equations (1), (2), (3), (4) the alignment energy of the hydrogen atom H as well as of the molecule H_2 has been calculated. The hydrogen alignment characteristics are presented in Table 1.

Table 1. The alignment characteristics of hydrogen atom H and molecule H_2

Hydrogen	Mass (Da)	Unaligned R	Aligned R	Alignment energy (eV)	Alignment energy difference (eV)
H	1,007825	3117,070 212	3117,001 583	11,250 881 313	
H_2	2,015650	6234,140 423	6234,000 792	11,445 545 701	0,194 664 388

e^-	0,00054857990907

We can see in Table 1 that the alignment energy of the hydrogen molecule $W_{alignment}^{H2} = 11{,}445545701$ eV is a little greater than that of the hydrogen atom $W_{alignment}^{H} = 11{,}250881313$ eV yielding the next alignment energy difference:

$$\Delta W_{alignment}^{H2-H} = W_{alignment}^{H2} - W_{alignment}^{H} = 0{,}194\ 664\ 388 \text{ eV}. \qquad (5)$$

Such energy difference has the temperature equivalent of T = 2259,0 K and is available at the Liquid-Liquid Critical Point (LLCP) of hydrogen.

4. The Hydrogen Liquid-Liquid Critical Point (LLCP)

The hydrogen Liquid-Liquid Critical Point (LLCP) - where both liquids have the same physicochemical characteristics - is located between (2300 K, 77 GPa) and (2200 K, 81 GPa) as shown in the *P–T* phase diagram for liquid hydrogen in Figure 1 [10]:

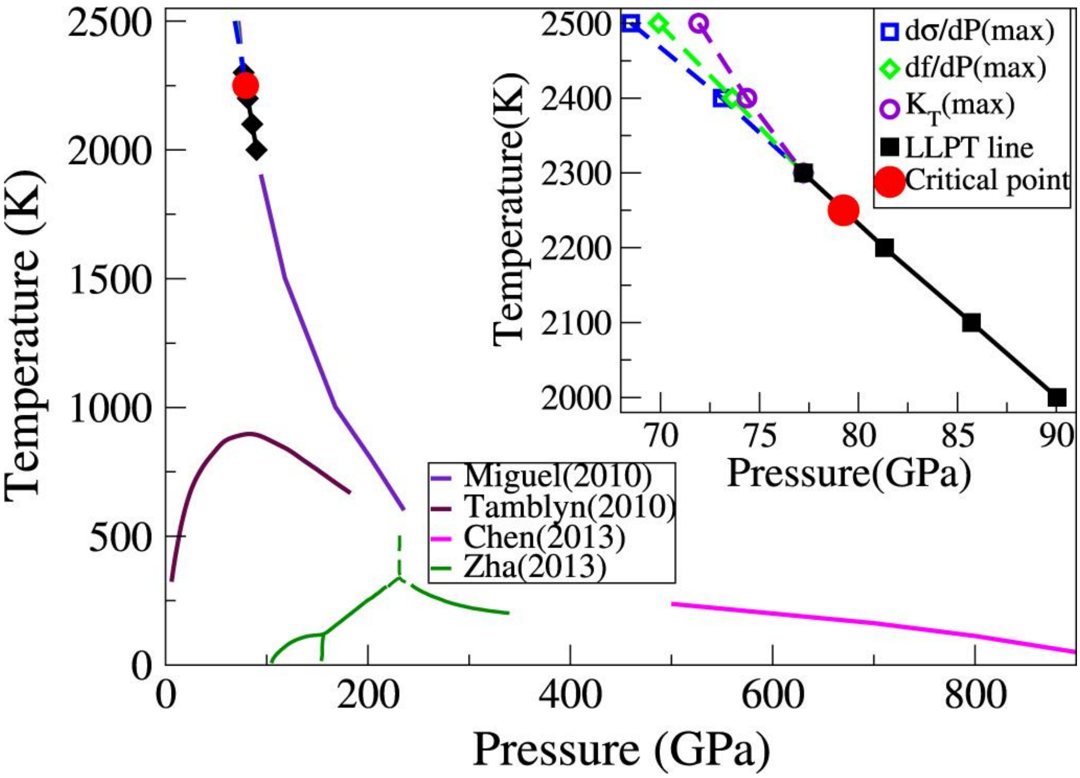

Figure 1 [10]**.** The *P–T* phase diagram for liquid hydrogen. As shown in the inset, the loci of different response function maxima, $\kappa_T^{\max}$ (open circle), $(d\sigma/dP)^{\max}$ (open square), $(df/dP)^{\max}$ (open diamond), are different. This difference in pressure along each isotherm for two continuous transitions, metal-to-insulator and molecular-to-atomic, becomes smaller and disappears as the liquid–liquid critical point (filled circle) is approached from the supercritical region, at which the peak of the response function maxima also diverge. Thus we can locate the LLCP of hydrogen by tracing the converging of response function extrema from the supercritical region. Below the LLCP, the response functions (e.g., κ_T, $d\sigma/dP$, df/dP) diverge as the first-order Liquid-Liquid Phase Transition (LLPT) line (filled square) is crossed. We note that melting curves below 200 GPa (brown curve) and above 500 GPa (pink curve) are from [11] and [12]. The LLPT line (violet curve) is from [13]. Phase boundaries between different phases (green curve) are from [14].

5. Conclusion

It seems that the difference between the hydrogen molecule and hydrogen atom alignment energy somehow determines the temperature of the liquid-liquid critical point (LLCP).

Dedication

This fragment was written on September 1, 2021 and is dedicated to the authors of Figure 1 as well as the 14 years of the Springer Pharmacy (Lekarna Špringer)

Figure2. *And yet it spins*

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