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Temperature Variation of Second Virial Coefficient and Viscosity for Deuterium (D_2)

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ABSTRACT
The Lennard-Jones potential is used to calculate the second virial coefficients of deuterium which agrees very well with experimental results at higher temperature (T≥360(K)) and use it to obtain Boyle's temperature. It is also use to calculate the viscosity of the deuterium as a function of temperature.
Keywords *Second Virial Coefficient, Interaction energy, viscosity, Lennard-Jones potential.*

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INTRODUCTION

The aim of this paper is to calculate theoretical estimates values of temperature-dependent second virial coefficient for deuterium which compares well with the experimental results. The Lennard-Jones potential as given in (2.1), and use it to obtain a temperature at which the force is exactly cancel. The good agreements of the computed values of viscosity are found to be with reported values.

SECOND VIRIAL COEFFICIENT: BRIEF DESCRIPTION OF THE THEORETICAL BACKGROUND

The equation of state of a gas may be expressed in terms of virial expansion, which is given by

$$P= \rho RT [1+B (T) \rho +C (T) \rho^2 +D (T) \rho^3 +\ldots\ldots\ldots\ldots \quad (1)$$

where P, R, T, and ρ are known as pressure, gas constant, temperature, and density respectively [13] and the coefficients B (T) & C (T) in the expression (1) are called the second and third. virial coefficients [6] and so on. The Lennard-Jones potential is perhaps most common form of potential energy and represents the non-bonded interaction between two molecules. In equation (2), the first term in the potential is repulsive force term and second term represents the attractive force term [15, 10]. For specific case of L-J (6-12) model the intermolecular potential energy and the corresponding intermolecular force [9] are giver by.

$$U(r) = 4\varepsilon[\left(\frac{\sigma}{r}\right)^{12} \quad \left(\frac{\sigma}{r}\right)^{6}] \quad (2)$$

$$F(r) = \quad dU(r)/dr \quad (3)$$

$$F(r) = 24\varepsilon/\sigma[2\left(\frac{\sigma}{r}\right)^{13} \quad \left(\frac{\sigma}{r}\right)^{7}] \quad (4)$$

In the above equations, r is the intermolecular separation, σ is the value of r for which the Lennard-Jones potential U(r) = 0, ε is the maximum energy of attraction (or depth of the potential wall) which occurs at r = $2^{1/6}\sigma$ [14]. Where ε *and* $\sigma$the parameters of the L-J potential and the best fit potential curve is shown in figure1 for deuterium. A simple expression for the second virial coefficient has been given by equation (16) [1, 2] which can be written as.

$$B(T) = 2\pi N_A 10^{-24} \int_0^\infty r^2 \left(1 \quad exp\left(\frac{U(r)}{kT}\right)\right) dr. \quad (5)$$

where Avogadro's Constant $N_A = 6.02 \times 10^{23}$, Boltzmann's Constant k_B= 1.3807x10 $^{-23}$(J.K^{-1}) and T is the temperature in Kelvin. Therefore we take the numerical values for deuterium from [12], which are$\frac{\varepsilon}{k} = 37.00\ (K), \sigma = 2.928(A^0)$. The variation of B(T) with temperature along with experiment values is

shown in figure 2. The calculated values of B(T) from (5) are displayed in table1for the temperature range 84K to 420K.

Logic of the temperature,where value of the B(T) is minimum

-Input values $(\frac{\varepsilon}{k_B})$ *and* σ (Å) in Mathmatica programme.

-Input Equation int[r_] = ((2Pi .602)(1 $e^{-4\ \frac{\varepsilon}{k_B}\ (\frac{1}{T})((\frac{\sigma}{r})^{12}-(\frac{\sigma}{r})^{6})}$ r^2); into wolfram Mathmatica 9.0 programme

- Calculate minimum value of temperature

For example, numerical evaluation of temperature for D_2.

$\frac{\varepsilon}{k_B} = 37.00(K), \sigma = 2.928(Å)$

In[1]: = int[r_] = ((2Pi .602)(1 $e^{-4\ 37.00\ (\frac{1}{T})((\frac{2.928}{r})^{12}-(\frac{2.928}{r})^{6})}$ r^2);

$B[T\_] = \text{Integrate}[\text{int}[r], \{r, 0, \infty\}, \text{Assumptions} \quad \{T \in \text{Reals}, T > 0\}]$

$\text{FindRoot}[B[T] = 0, \{T, 600\}]$

Out[2]=

$$\frac{135.3294492895741\sqrt{T}\text{Hypergeometric1F1}[-0.25,0.5,\frac{37.00000000000004}{T}]-1217.7565113672567\text{Hypergeometric1F1}[0.25,1.5,\frac{37.00000000000004}{T}]}{T^{3/4}}$$

Out[3]= $\{T \to 126.463\}$

VISCOSITY

The Chapman-Enskog solution of the Boltzmann equation provided one with a formally complete solution of the problem of interpreting the transport properties of matter. The particular, one obtains phenomenological flow equation to the intermolecular potential function. The viscosity expression (in g/cm sec) for deuterium D_2 as function of temperature [7] is given by

$$\eta \times 10^7 = 266.93\ (MT)^{1/2} / \sigma^2\ \Omega^{(2,2)^*}\ T^* \qquad (6)$$

where M = molecular weight, T = absolute temperature, σ = collision diameter of a molecule in Å and $\Omega^{(2,2)^*}$ is the collision integral which is a function of reduced temperature T* [6] by

$$\Omega^{(2,2)^*}\ T^* = 1.147\ (T^*)^{-0.145} + (T^* + 0.5)^{-2} \qquad (7)$$

Where T* is the reduce temperature which is defined as T* = k T/ε and ε is the Lennard-Jones Potential well depth [3]. The theoretical curve of such a comparison is shown in figure3 and computed values based upon the Lennard-Jones potential are also listed in table1. The calculated values of viscosity are found to be in very good agreement with the observed values [8] as shown in figure3. The percentage error in the temperature range 84(K) to 273.15(K) is ±3.09% and the population standard deviation is 1.89. At higher temperatures (T ≥ 300 (K)) upto 420(K) the viscosity uncertainty as a population standard deviation is 0.408 and it is found that the approximate numerical error is ±0.73% at the above temperature range. As described [8 at pp.191], at higher temperature (upto 2200(K)), the overall error should be no more than ±4%. The experimental data depart from the correlation by no more than ±0.7% over the entire temperature range.

RESULT AND DISCUSSION

In general, the thermodynamic and transport properties of normal fluids may be expressed by using the Lennard-Jones (6-12) potential. In this paper, we are focusing especially on the Lennard-Jones intermolecular potential for the computations of D_2 properties. The Lennard-Jones potential is a theoretical model to calculate the approximate interaction energy between molecules. The total potential energy of interaction between two molecules is based on Lennard-Jones potential function and may be calculated from equation (2) [16]. Thus its formulation fitted curve is shown in fig.1.

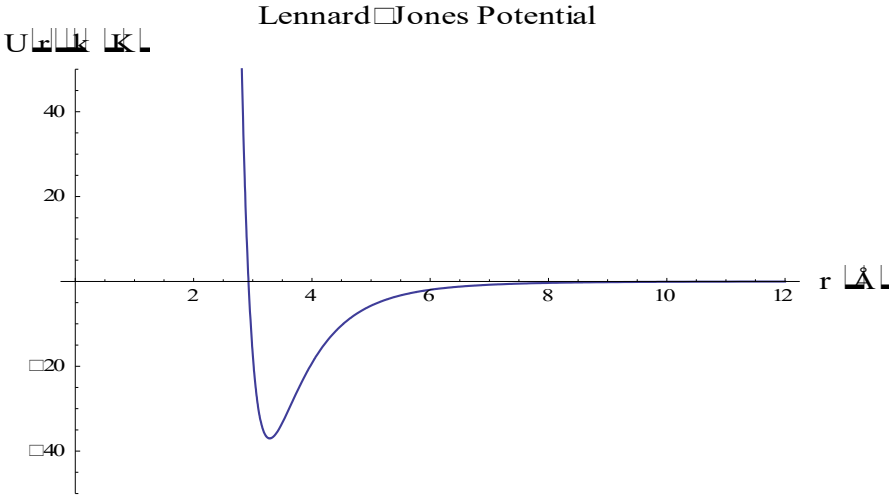

Figure1. Potential energy U(r)/k versus separation r(Å)for D_2 as [2]

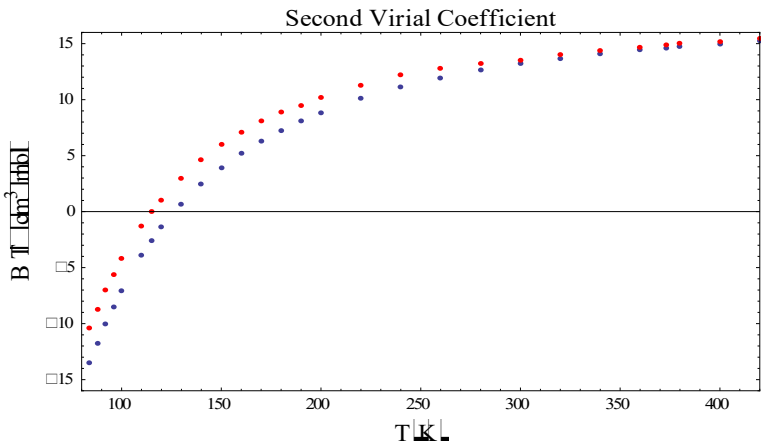

Figure 2.Second virial coefficient B (T) verses Temperature T (K) for D_2.Exp, blue [4] and cal. (red).

$\eta \times 10^7$	T(K)	$B^{[4]}_{Exp.}(T)$	$B_{Cal.}(T)$	%difference
498.067	84.00	-10.4	-13.85	33.17
535.956	92.00	-7.0	-10.10	44.28
572.457	100.00	-4.2	-7.04	67.61
616.343	110.00	-1.3	-3.92	201.53
658.515	120.00	1.0	-1.39	239
699.171	130.00	3.0	0.69	77
738.479	140.00	4.6	2.44	46.95
776.58	150.00	6.0	3.93	34.5
813.595	160.00	7.1	5.20	26.76
849.626	170.00	8.1	6.30	22.22
884.762	180.00	8.9	7.26	18.42
919.078	190.00	9.5	8.11	14.63
952.642	200.00	10.2	8.85	13.23
1017.74	220.00	11.3	10.11	10.53
1080.43	240.00	12.2	11.12	8.85
1141.03	260.00	12.8	11.94	6.71
1179.97	273.15	13.1	12.40	5.3
1199.78	280.00	13.2	12.62	4.39
1256.87	300.00	13.5	13.19	2.22
1312.49	320.00	14.0	13.67	2.35
1366.76	340.00	14.4	14.08	2.22
1419.8	360.00	14.7	14.43	1.83
1454.16	373.15	14.9	14.63	1.81
1471.72	380.00	15.0	14.73	1.8
1522.6	400.00	15.2	14.99	1.38
1572.51	420.00	15.5	15.22	1.80

Table1. Comparison of calculated and experimental values of B(T) and viscosity with T(K) of D_2.

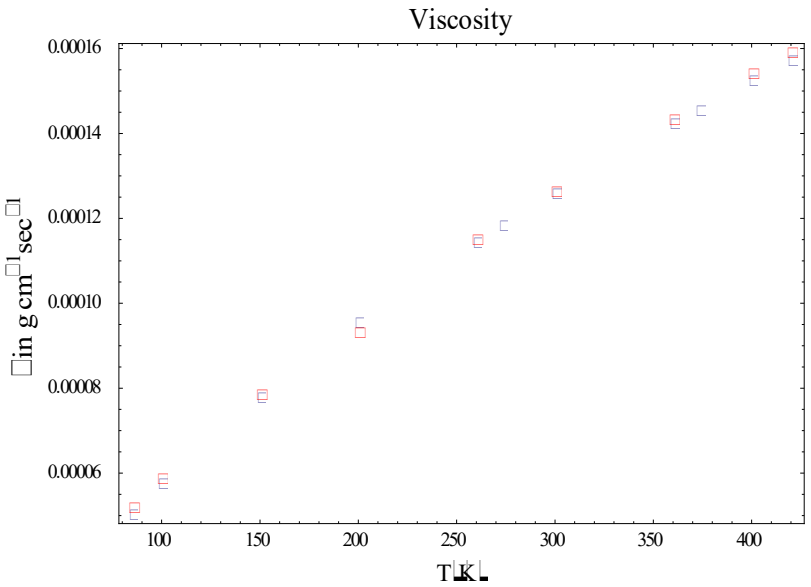

Figure 3. Coefficient of viscosity v/s temperature (in kelvin) of deuterium D_2. As reported, red [8] and cal. (blue).

The numerical values of second virial coefficient B(T) can be carried out by equation (5) it is necessary to know the values of the force constants, ε and σ appropriate for the given substance. The calculated values as a numerical comparison is made in table 1 as a function of temperature. The Lennard-Jones potential parameters are used to compute the second virial coefficient of D_2 which agrees with experimental results particularly at higher temperature (T ≥ 360(K)) upto 420(K), as shown in fig.2. There is a large discrepancy at lower temperatures (T≤ 126.463(K)), the second virial coefficients B(T) is negative, where the attractive part of the interaction potential for molecule is dominates. At high temperature (T ≥ 126.464(K)), there is a good agreement between experimental and calculated results and at this temperature, the second virial coefficients B(T) is dominated by the repulsive force and is, consequently positive. A temperature will exist at which the force exactly cancel and B(T)=0; [11] this is called the Boyle's temperature T_B. At temperature T= 126.463(K), the value of B(T) is -0.0000684168(cm^3/mol) and at T=126.462(K), the value of B(T)is -0.000271525 (cm^3/mol). The Lennard-Jones parameters are used to calculate the minimum value of B(T) by using the wolfram mathmatica 9.0 as follow; $T_B \approx 126.464$ (K), B(T) ≈ 0.000134688(cm^3/mol).

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