

Modified van der Waals Gas Equation Derived from Experimental Data of Xenon

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Abstract

The original version of the van der Waals gas equation of state has been modified in order to obtain second and third virial coefficients that match experimental results for the noble gas xenon. This modified version of the van der Waals equation shows that even a noble gas such as xenon displays surprisingly quite complicated behavior. Proper modifications of the van der Waals equation were performed from the utilization of empirical data of xenon and also from computer simulations of xenon atoms using the hard-sphere potential. The empirical data of xenon employed were the measured liquid and vapor molar volumes, the measured liquid-vapor equilibrium pressure values, the measured critical point data (the measured critical pressure, temperature and molar volume), and experimental high pressure results acquired at temperatures above the measured critical temperature value of 289.7 Kelvin. Also, correct modifications reveal that clustering effects or the formation of van der Waals molecules are in particularly important near and below the critical temperature value.

The Original van der Waals Gas Equation

The original version of the van der Waals gas equation was developed by J. D. van der Waals during the late 19th century [1], and this was the first equation of state formulated for modeling real gases and liquids. The following expression represents the first version of the van der Waals gas equation with constant a_2 - and b -parameters:

$$P = RT/(v - b) - a_2/v^2 \quad (1)$$

The b -parameter, or the effective atomic or molecular molar volume of a gas, constitutes the limited volume of space occupied by gaseous atoms or molecules since atoms are not point masses, and this parameter likewise represents the highly repulsive forces that occur during atomic or molecular collisions for a real gas. This enhances the pressure of a real gas as compared to that of an ideal gas composed of non-interacting point-mass atoms. Conversely, the a_2 -parameter simulates the attractive two-body interactions between atoms or molecules when they are separated in space. The attractive force, between any two gaseous atoms or molecules, decrease as their separation distance increases. To simulate this effect, the a_2 -parameter is divided by the gas molar volume ($v = V/n$) raised to the second power.

From differential calculus techniques and the critical point definition [2], parameters a_2 and b , in the original version of the van der Waals equation of state, are derived to be the following functions of the measured critical temperature T_c and measured critical pressure P_c :

$$a_2 = (27/64) R_c^2 T_c^2 / P_c \quad (2)$$

$$b = (1/8) R T_c / P_c \quad (3)$$

Traditionally, these two parameters in the van der Waals gas equation are assumed to be constant, modeling the dual existence of the liquid and vapor phases of matter for any pure substance at temperatures below the critical temperature value. However, when keeping these two parameters constant, the van der Waals equation of state poorly models real gases and liquids quantitatively. For example, when using the parameter values calculated from Equations 2 and 3, the critical molar volume value v_c of the original van der Waals equation is usually larger in value than that observed experimentally. For xenon, the measured critical molar volume is 0.1194 Liter/mole [3] but the value from the original van der Waals equation is 0.1552 Liter/mole, a factor of 1.300 times larger than that observed experimentally.

Concerning the poor quantitative modeling of real gases by the original van der Waals gas equation, the second and third virial coefficients derived from the van der Waals equation badly match the experimental curves of these two coefficients (Figures 1 and 2). When deriving the virial expansion of the compressibility factor Z for a real gas:

$$Z = P v / (R T) = 1 + B / v + C / v^2 + D / v^3 + \dots \quad (4)$$

Using the traditional van der Waals expression results in the following infinite series:

$$Z = P v / (R T) = 1 + [b - a_2 / (R T)] (1/v) + b^2 / v^2 + \dots \quad (5)$$

The second virial coefficient B and third virial coefficient C in terms of the traditional van der Waals gas equation are, therefore:

$$B = b - a_2 / (R T) \quad (6)$$

$$C = b^2 \quad (7)$$

Respectively, Figure 1 and Figure 2 display the expressions in Equations 6 and 7 along with the experimental temperature curves [4] of the second and third virial coefficients of xenon. The worse discrepancy is that for the third virial coefficient. The simple van der Waals expression predicts that the third virial coefficient is constant which is extremely far removed from what has been observed experimentally for real gases in general. Therefore, the behavior of a real gas is much more complex than that demonstrated by the original van der Waals equation of state. For example, the b -parameter in the van der Waals gas, or the effective atomic or molecular molar volume b for any real gas, should definitely have dependence upon the gas molar density ($\rho = 1/v$), the reciprocal of the gas molar volume v , and upon the absolute temperature T as well.

The Dependence of the b -Parameter upon the Gas Molar Density

In the hard-sphere model, the effective atomic or molecular gas molar volume b is independent of the temperature but definitely dependent upon the gas molar density $1/v$. Thus, the first step in rectifying the simple van der Waals gas equation was the employment of computer simulations for determining the b -parameter dependence upon the gas molar density. To accomplish this task, the noble gas xenon was modeled utilizing the hard-sphere potential. For the hard-sphere potential, the following expression applies to the pressure since there are no attractive interactions taking place, just only the highly repulsive interactions during collisions between two gas atoms or molecules:

$$P = RT/(v - b_{\text{HS}}) \quad (8)$$

A substantial number of simulations were performed for one-thousand or more xenon gas atoms, contained within a hypothetical cubic gas volume at specific temperatures and molar volumes. For every simulation, the values b_{HS} of the b -parameter in the hard-sphere potential were computed from the observed simulation pressure values P at the six flat walls of the cubic gas volume. Also, in each simulation at the very beginning, the simple cubic unit cell arrangement was utilized to initially position the atoms with the atomic separation distances being established by the input of a specific molar density. Then a Gaussian random number generator [5] was utilized so the xenon gas atoms in the computer simulation would have the Maxwellian velocity distribution. Figure 3 displays the results from the computer simulations of xenon, where the abscissa is the ratio of b_{HS} and b_{AV} , with b_{AV} being equal to the total volume occupied by one mole of hard-spheres, each hard-sphere having an atomic volume v_a :

$$b_{\text{AV}} = N_A v_a = N_A (4\pi/3) (\sigma/2)^3 \quad (9)$$

In Equation 9, N_A is Avogadro's number and σ is the diameter of the hard-sphere, which is set equal to the σ -parameter of the Lennard-Jones potential obtained from viscosity data [2]. Theoretically in the limit of zero molar density of a gas composed of hard-spheres, the effective molar atomic volume for one mole of the hard-sphere gas atoms is exactly equal to four times the expression in Equation 9 [1]. The most appropriate fit to the simulation data points in Figure 3 is the following equation of a hyperbola, reaching a minimum value of 2 at the maximum density and a maximum value of 4 at zero molar density:

$$b_{\text{HS}}/b_{\text{AV}} = 1 + \{ 1 + 2(4b_{\text{AV}})^2 [1/v - 2/(4b_{\text{AV}})]^2 \}^{1/2} \quad (10)$$

Hence, when applying the first correction to the traditional van der Waals equation of state, the original constant b -parameter was substituted by the following equation of a hyperbola where the gas molar density, $1/v$, is the independent variable:

$$b = (b_0/4) \{ 1 + [1 + 2b_0^2 (1/v - 2/b_0)^2]^{1/2} \} \quad (11)$$

In Equation 11, the b_0 -parameter represents four times the total volume occupied by one mole of individual gaseous atoms or molecules:

$$b_0 = 4 b_{AV} = 4 N_A v_a \quad (12)$$

When substituting Equation 11 for the b -parameter in the original van der Waals equation, the two parameters to be evaluated are b_0 and a_2 . From techniques of differential calculus and the critical point definition, these two parameters are the following functions of the measured critical temperature and pressure values:

$$b_0 = (R T_c / P_c) / 5.557586863 \quad (13)$$

$$a_2 = (R^2 T_c^2 / P_c) / 2.04504859 \quad (14)$$

These two formulas are slightly different from the expressions in Equations 2 and 3. In addition, when substituting the expression in Equation 11 into the original van der Waals expression, the calculated critical molar volume for xenon is 0.1480 Liter/mole which is smaller in value than that from the traditional van der Waals expression, but this value is still larger than that observed experimentally by a factor of 1.240. Apparently for a real gas, the value of the b_0 -parameter must have dependence upon the gas molar density as does the b -parameter.

With regards to the virial expansion when utilizing this first modification of the van der Waals equation, the second virial coefficient is exactly the same expression as before (Equation 6), but the numerical value of the a_2 -parameter will be different, and the numerical b_0 -parameter value will also be different from that of the constant b -parameter value in the original van der Waals expression:

$$B = b_0 - a_2 / (RT) \quad (15)$$

Concerning the third virial coefficient, it still comes out as a constant but is likewise a different constant value from the situation with the original van der Waals expression:

$$C = (2/3) b_0^2 \quad (16)$$

Surprisingly at temperatures above the critical temperature value, the second virial coefficient matches experimental data closer when substituting the van der Waals b -parameter with Equation 11 (Figure 4). Also, from observing Figure 4 for temperatures above the critical value ($T_c = 289.7$ K [3]), the value of the a_2 -parameter may be assumed to be independent of temperature and constant. Yet, concerning the match between experiment and the third virial coefficient (Figure 5), this first modification of the van der Waals equation results in a poorer fit at high temperatures.

In theory, the third virial coefficient as well as the second virial coefficient approach negative infinity within the limit of absolute zero. To accomplish this, it would be necessary to insert an a_3 -coefficient into the van der Waals equation as well as

substitution of Equation 11 into the b -parameter for the original van der Waals expression:

$$P = RT/(v - b) - a_2/v^2 - a_3/v^3 \quad (17)$$

Now there are three parameters to match with the three measurable data at the critical point of a pure substance:

$$\text{Parameters: } b_0, a_2, \text{ and } a_3 \quad \text{Measurable Data: } T_c, P_c, \text{ and } v_c$$

Then with the inclusion of the a_3 coefficient, the third virial coefficient becomes the following expression:

$$C = (2/3) b_0^2 - a_3/(RT) \quad (18)$$

However, when utilizing the measured critical point data [3] for xenon gas:

$$T_c = 289.7 \text{ Kelvin}$$

$$P_c = 58.21 \text{ Atmospheres}$$

$$v_c = 0.1194 \text{ Liter/Mole}$$

The corresponding van der Waals three parameters have the following bizarre values:

$$b_0 = -0.1284 \text{ Liter/Mole}$$

$$a_2 = 0.6787 \text{ Atmospheres (Liter/Mole)}^2$$

$$a_3 = -0.04289 \text{ Atmospheres (Liter/Mole)}^3$$

The negative b_0 -parameter in reality does not make any physical sense, and if one utilizes Equation 15 for evaluation of the second virial coefficient $B(T)$, there would be a very poor match with experimental observations. Also, the negative value of the a_3 -parameter results in the third virial coefficient becoming infinitely positive rather than infinitely negative in the limit of absolute zero, which is contradictory to experiment as well as theory. These results from the addition of the a_3 -parameter into the van der Waals equation along with the constant b_0 -parameter show that something is missing for a correct model of real gases. In addition, the experimentally observed third virial coefficient curve complexity (Figure 5), as well as that for the second virial coefficient at low temperatures (Figure 4), reveals that the b_0 -parameter must be a function of temperature as well as molar density.

b_0 Dependence upon Temperature and Molar Density for Constant a_2 and a_3

To determine the dependence of the b_0 -parameter upon the molar density and temperature of a real gas, the b_0 -parameter in the modified van der Waals equation was carefully analyzed using experimental high pressure data [3] of xenon gas obtained at different temperatures. Figure 6 displays the experimental values of the b_0 -parameter acquired at different pressures (from 100 to 1,000 bars in steps of 100 bars) at 500 Kelvin. The plot of experimental b_0 -parameter values versus the gas molar density at 500 Kelvin matches the following negative exponential function of the gas molar density ($1/v$):

$$b_0 = c_0 + c_1 \exp(-k_1 / v) \quad (19)$$

Assuming the predetermined numerical values of the a_2 and a_3 coefficients are constant, this analysis was performed for all experimental xenon gas high pressure data obtained at temperatures from 300 Kelvin to 1,000 Kelvin in steps of 100 Kelvin. The results were consistent with the negative exponential as an appropriate fit for the dependence of the b_0 -parameter upon the gas molar density. However, the determined numerical values of the c_0 -, c_1 -, and k_1 -parameters acquired from curve-fitting the high pressure data obtained at different temperatures varied with the temperature (Figures 7 to 9). One physical interpretation of this negative exponential function in Equation 19 is that with increasing molar density, or decreasing molar volume, there is increasing atomic electron cloud overlap from increasing atomic collision frequency, resulting in a decrease of the b_0 -parameter with increasing molar density. Also, another interpretation is that due to the short-range attractive forces between two atoms in the gaseous phase, atoms may appear slightly smaller in size because of decreasing velocity as two atoms move further apart at concentrated molar densities.

Nonetheless, in accomplishing this result it was initially necessary to predetermine appropriate numerical values for the a_2 and a_3 coefficients. This was achieved by the evaluation of the c_0 -, c_1 -, and k_1 -parameters in Equation 19 at the critical point using the measured critical molar volume v_c as well as the measured critical pressure P_c and critical temperature T_c . Also, the experimental third virial coefficient value $C(T_c)$ at the critical temperature [4] was used for determining the numerical value of the a_3 coefficient. Concerning the a_2 coefficient, an appropriate value was used which yielded second and third virial coefficients that best match the experimental curves keeping a_2 and a_3 coefficients constant. For the modified van der Waals equation with the inclusion of the a_3 coefficient and incorporation of Equations 11 and 19, the second and third virial coefficients become:

$$B = (c_0 + c_1) - a_2 / (RT) \quad (20)$$

$$C = (2/3) (c_0 + c_1)^2 - k_1 c_1 - a_3 / (RT) \quad (21)$$

And the best numerical value of the a_2 coefficient utilized is given by the following expression:

$$a_2 = 1.40 (R^2 T_c^2 / P_c) / 2.04504859 \quad (22)$$

1.40 times the value derived in Equation 14. Another very important result is that the a_3 coefficient value is around two orders of magnitude less than that of the a_2 coefficient, representing a rapidly converging series, and so, it is feasible to neglect a_4 and higher order terms.

On the other hand, at temperatures below the critical temperature value in the liquid-vapor region of xenon, the values of the c_0 -, c_1 -, and k_1 -parameters were determined at different temperatures using the theory [1] that the molar Gibbs free energies of a liquid and the vapor of a pure substance are equal at the measured equilibrium liquid-vapor pressure value. This incorporated the use of the experimental equilibrium liquid-vapor pressure P_{equil} at a specific temperature and corresponding measured liquid molar volume v_l and vapor molar volume v_g . Thus, the following mathematical expression was used to evaluate the c_0 -, c_1 -, and k_1 -parameters at a specific temperature value:

$$P_{\text{equil}} (v_g - v_l) = \int_{v_l}^{v_g} P dv \quad (23)$$

Also, if one assumes that the a_2 and a_3 coefficients are constant, the evaluated b_0 -parameters from the measured liquid and vapor molar volumes at different temperatures yield a b_0 -curvature (Figure 10) not consistent with that observed for high pressure data above the critical temperature value (Figure 6) when using Equations 11 and 17. The observed decrease in the b_0 -parameter at low molar densities in Figure 10, for vapor molar volumes close to the melting point, is not likely due to any real decrease in the b_0 -parameter with increasing molar volume and decreasing molar density. Instead, this observed decrease is more likely due to the formation of van der Waals molecules or clusters, resulting in a slight decrease in the number of gaseous particles. Thus, an f multiplication factor was incorporated as an additional modification of the van der Waals equation for temperatures below the critical temperature value:

$$P = f R T / (v - b) - a_2 / v^2 - a_3 / v^3 \quad (24)$$

Evaluation of f as a Function of Temperature and Molar Density

At and above the critical temperature, the f multiplication factor is nearly equal to one. Because of clustering effects decreasing the total number of gaseous particles in the vapor phase at lower temperatures, the f multiplication factor would have a value slightly less than one. In order to match the experimental curves for the second and third virial coefficients of xenon at lower temperatures, the following negative exponential function was assumed to properly model this f multiplication factor which includes two additional parameters c_2 and k_2 :

$$f = 1 - (c_2 / v) \exp(-k_2 / v^2) \quad (25)$$

The c_2 -parameter value can be determined by evaluating the f multiplication factor when assuming that Equation 19 applies to the b_0 -parameter dependence upon molar density. But when evaluating the numerical value of the k_2 -parameter, the minimum value of the f factor is assumed to occur at or near the maximum pressure value between the liquid and vapor molar volumes (Figure 11). For the liquid-vapor region of xenon, Figure 12 and Figure 13 display the temperature variation of the c_2 - and k_2 -parameters, and both curves nearly match that of a negative exponential decay function for the absolute temperature:

$$c_2 = c_{2,0} \exp(-\lambda_c T) \quad (26)$$

$$k_2 = k_{2,0} \exp(-\lambda_k T) \quad (27)$$

And from the results of Figure 12 and Figure 13, the c_2 - and k_2 -parameters are not exactly equal to zero at the critical temperature, but instead close to zero and rapidly approach zero with increasing temperatures beyond the critical temperature value. The numerical fits of Equations 26 and 27 can be utilized again to re-evaluate the values of the c_0 -, c_1 -, and k_1 -parameters for all temperature values of the liquid-vapor equilibrium data and high pressure data.

With the inclusion of Equation 25 into the modified van der Waals equation, the second and third virial coefficients now become the following two expressions:

$$B = (c_0 + c_1 - c_2) - a_2 / (RT) \quad (28)$$

$$C = (2/3) (c_0 + c_1)^2 - k_1 c_1 - c_2 (c_0 + c_1) - a_3 / (RT) \quad (29)$$

When using the evaluated values of the c_0 -, c_1 -, and k_1 -parameters, evaluated values of the constant a_2 - and a_3 -coefficients, and exponential fits for the c_2 - and k_2 -parameters, Equation 28 and Equation 29 display decent matches (Figure 14 and Figure 15) with the experimental second and third virial coefficients for xenon, respectively.

Conclusion

Thus far, it has been possible to modify the original van der Waals equation of state to match up with experimentally observed second and third virial coefficients for xenon:

$$P = fRT / (v - b) - a_2 / v^2 - a_3 / v^3 \quad (24)$$

$$f = 1 - (c_2 / v) \exp(-k_2 / v^2) \quad (25)$$

$$b = (b_0 / 4) \{ 1 + [1 + 2 b_0^2 (1/v - 2/b_0)^2]^{1/2} \} \quad (11)$$

$$b_0 = c_0 + c_1 \exp(-k_1 / v) \quad (19)$$

$$c_2 = c_{2,0} \exp(-\lambda_c T) \quad (26)$$

$$k_2 = k_{2,0} \exp(-\lambda_k T) \quad (27)$$

Concerning the c_0 -, c_1 -, and k_1 -parameters dependence upon temperature (Figures 7 to 9), peculiar discontinuities occur consistently at the measured critical temperature value of 289.7 Kelvin. For the c_0 -parameter, its numerical value is assumed to be constant at temperatures equal to and less than the critical temperature value ($T \leq T_c$). With regards to infinite pressures, this result causes the minimum molar volume v_{\min} at infinite pressures to vary slightly with temperature (Figure 16). The slight decrease in the minimum molar volume with temperature near the freezing point of xenon, 161.4 Kelvin, correlates with the solid phase having slightly higher density than the liquid phase.

At temperatures from 500 Kelvin and higher, the c_0 -, c_1 -, and k_1 -parameters temperature dependences are well modeled by the following inverse temperature relationships:

$$c_0 = C_0 / T^x \quad (30)$$

$$c_1 = C_1 / T^y \quad (31)$$

$$k_1 = K_1 / T^z \quad (32)$$

For the c_1 -parameter at temperatures below the critical temperature value (Figure 8), the following quadratic expression well matches the nearly quadratic temperature curve:

$$c_1 = \kappa_0 + \kappa_1 (T/T_c) + \kappa_2 (T/T_c)^2 \quad (33)$$

And for the k_1 -parameter below the critical temperature value (Figure 9), the following cubic function works best to model the temperature dependence:

$$k_1 = \gamma_0 + \gamma_1 (T/T_c) + \gamma_2 (T/T_c)^2 + \gamma_3 (T/T_c)^3 \quad (34)$$

One of the important final results is achieved by extrapolating the second virial coefficient of the modified van der Waals gas to extremely high temperatures utilizing Equations 30 and 31 as well as Equation 26 into the expression in Equation 28. This will yield a maximum in the second virial coefficient at a high temperature value nearly fifteen times the numerical value of the critical temperature which matches experimental studies [6] of real gases at very high temperatures (Figure 17).

In order to evaluate the values of the c_0 - and k_1 -parameters at temperatures between the measured critical temperature value, 289.7 Kelvin, and 500 Kelvin, due to the particular discontinuities at the critical temperature value one needs first to fit the second and third virial coefficient curves of the modified van der Waals expression by the following polynomials:

$$B = \beta_1 (T_c/T) + \beta_2 (T_c/T)^2 + \beta_3 (T_c/T)^3 + \dots \quad (35)$$

$$C = \eta_1 (T_c/T) + \eta_2 (T_c/T)^2 + \eta_3 (T_c/T)^3 + \dots \quad (36)$$

And the temperature of the c_1 -parameter between the critical temperature value and 400 Kelvin could be fitted with a nonlinear polynomial function similar to Equation 34. From these three separate functions, then the values for the c_0 - and k_1 -parameters could be evaluated between the critical temperature of 289.7 Kelvin and 500 Kelvin (Figures 18 and 19).

Evidently, this analysis of xenon gas shows that real gases in general display quite complex behavior. The critical point also is a point of discontinuity as well as the point where the first and second derivative of the pressure with respect to the molar volume is zero in the P , T , and v curvature. Also, when analyzing the dynamics of real gases that are polar covalent and also polar gases which involve hydrogen bonding, further modifications may be necessary. The future plan is to continue this investigation into the other noble gases and non-polar gases as well as polar.

Another complicated interesting aspect about the behavior of xenon gas is the schematic behavior for the b_0 -parameter as a function of the molar density at different constant temperatures. Figure 20 displays these results for xenon at and above the measured critical temperature value of 289.7 Kelvin using Equation 19 and the plotted parameters in Figures 7 to 9. The shapes of the curves follow a typical pattern from 400 to 1000 Kelvin. But at the critical temperature and 300 Kelvin, the schematics change. Near the critical temperature value, this may be an effect from overlapping of electron clouds between two or more atoms occurring at higher molar densities, resulting in a further decrease in the b_0 -parameter with increasing molar density.

Concerning the liquid-vapor region, Figure 21 displays the b_0 -parameter as a function of the molar density at and below the critical temperature value. The schematics remain nearly constant with increasing maxima in the curves with decreasing temperatures. This can be understood due to less atomic overlap in collision with dropping temperature values for any gas or vapor. However, with increasing molar density, all the curves in Figure 21 approach nearly the same value, which may be interpreted to the formation of the liquid phase where there is nearly a constant quantity of atomic electron cloud overlaps.

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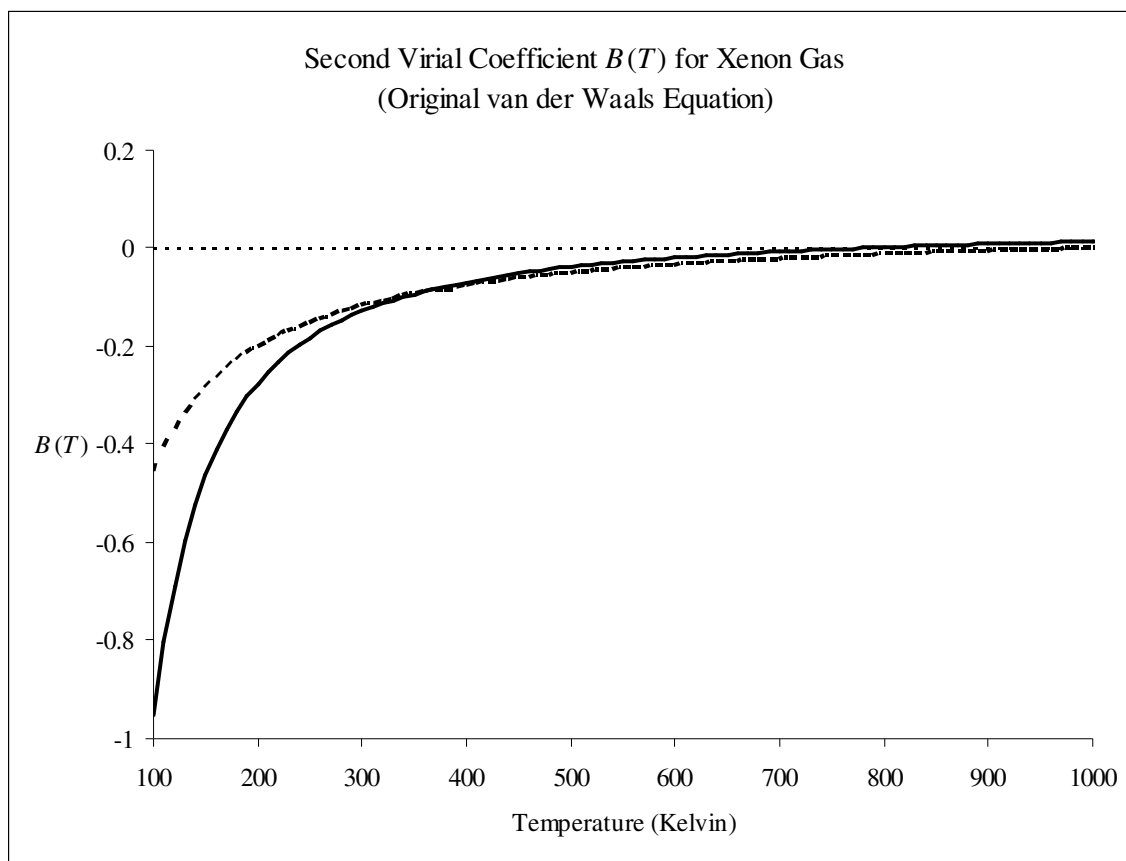


Figure 1 The second virial coefficient for xenon gas

The solid curve represents experimental result and the dash-curve is from the original van der Waals gas equation.

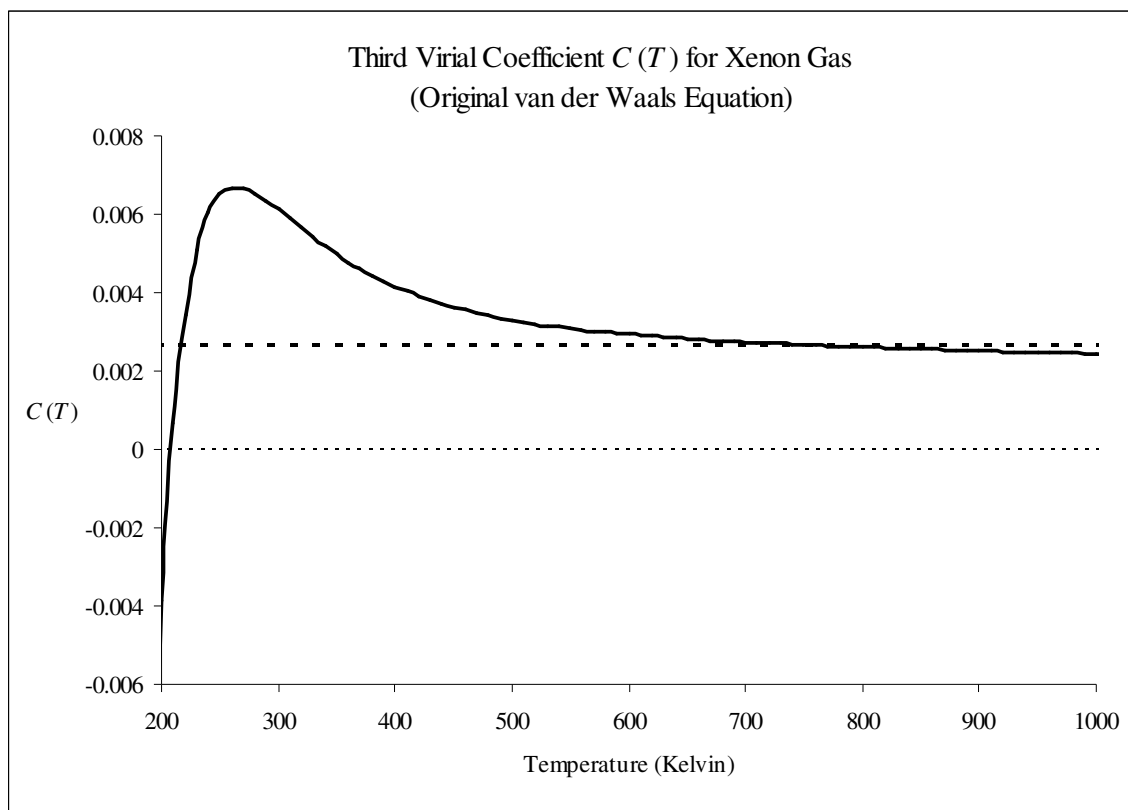


Figure 2 The third virial coefficient for xenon

The solid curve represents experimental result and the dash-curve is from the original van der Waals gas equation.

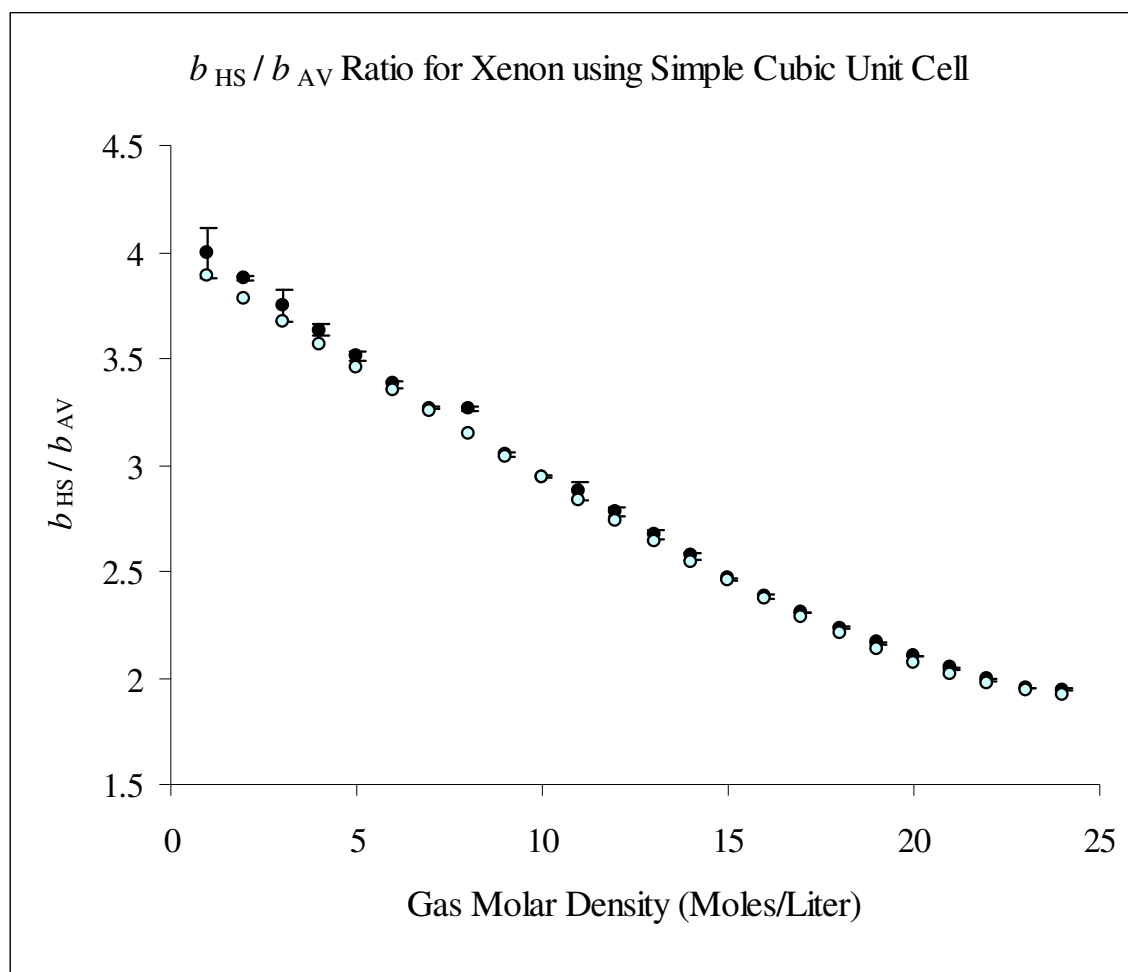


Figure 3 Molecular dynamics computer simulation results for the b -parameter of the van der Waals gas equation utilizing the hard-sphere model

The filled-in circles are the results from computer simulations, and the open-circles are from the following equation of a hyperbola as a function of the molar density ($1/v$):

$$b_{HS} / b_{AV} = 1 + \{ 1 + 2 (4 b_{AV})^2 [1/v - 2/(4 b_{AV})]^2 \}^{1/2}$$

$$b_{AV} = N_A v_a = N_A (4\pi/3) (\sigma/2)^3$$

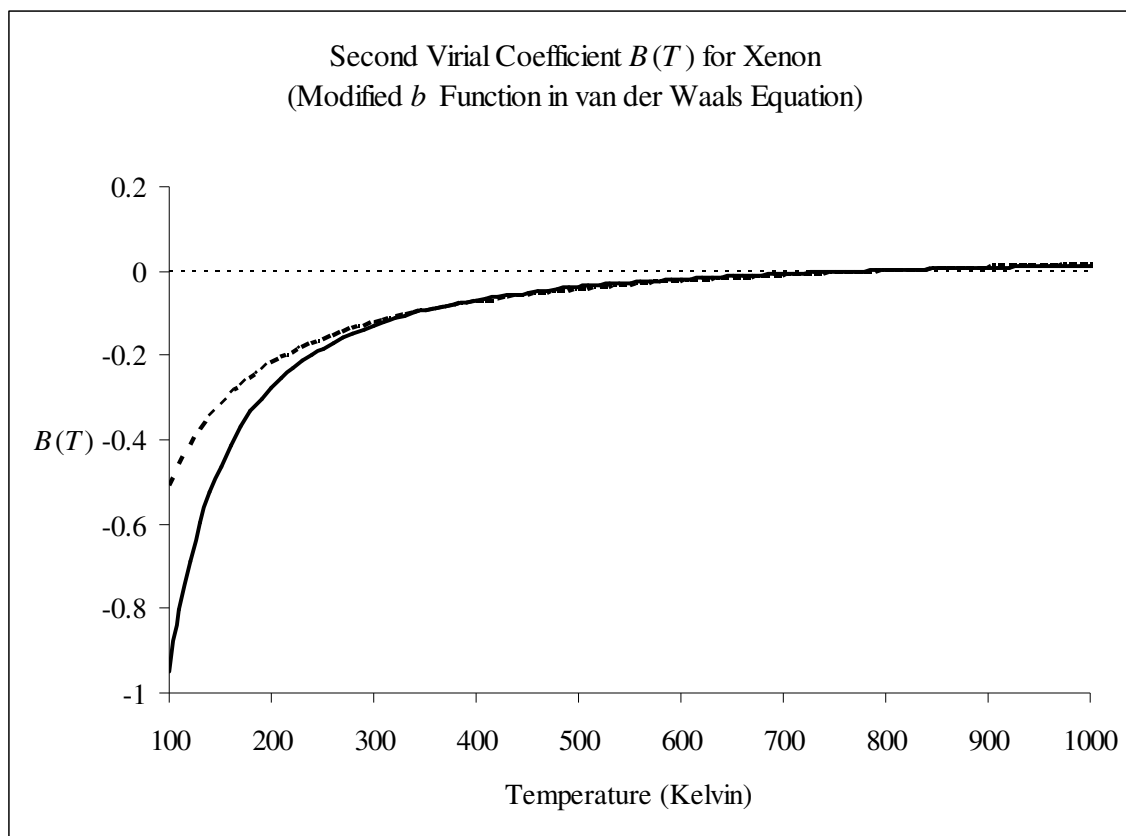


Figure 4 The second virial coefficient for xenon in units of Liter/mole

The solid curve represents experimental result and the dash-curve is from the van der Waals gas equation modified for the b -parameter only.

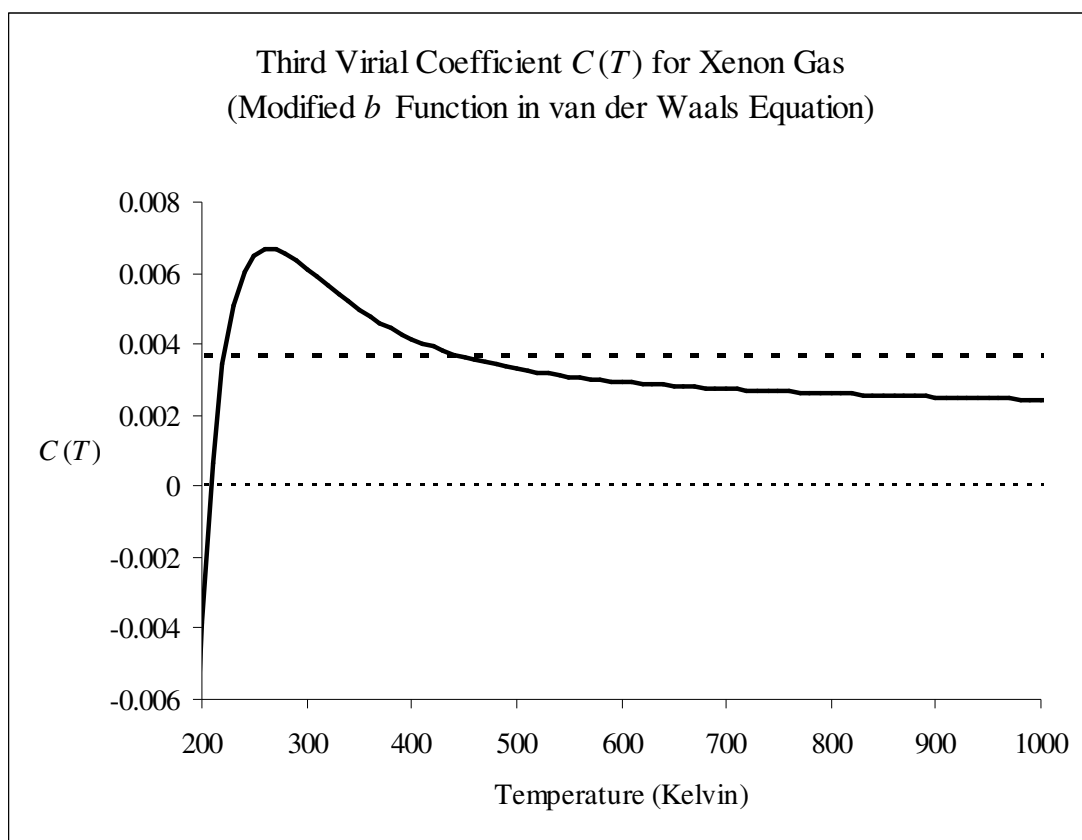


Figure 5 The third virial coefficient for xenon in units of Liter²/mole²

The solid curve represents experimental result and the dash-curve is from the van der Waals gas equation modified for the b -parameter only.

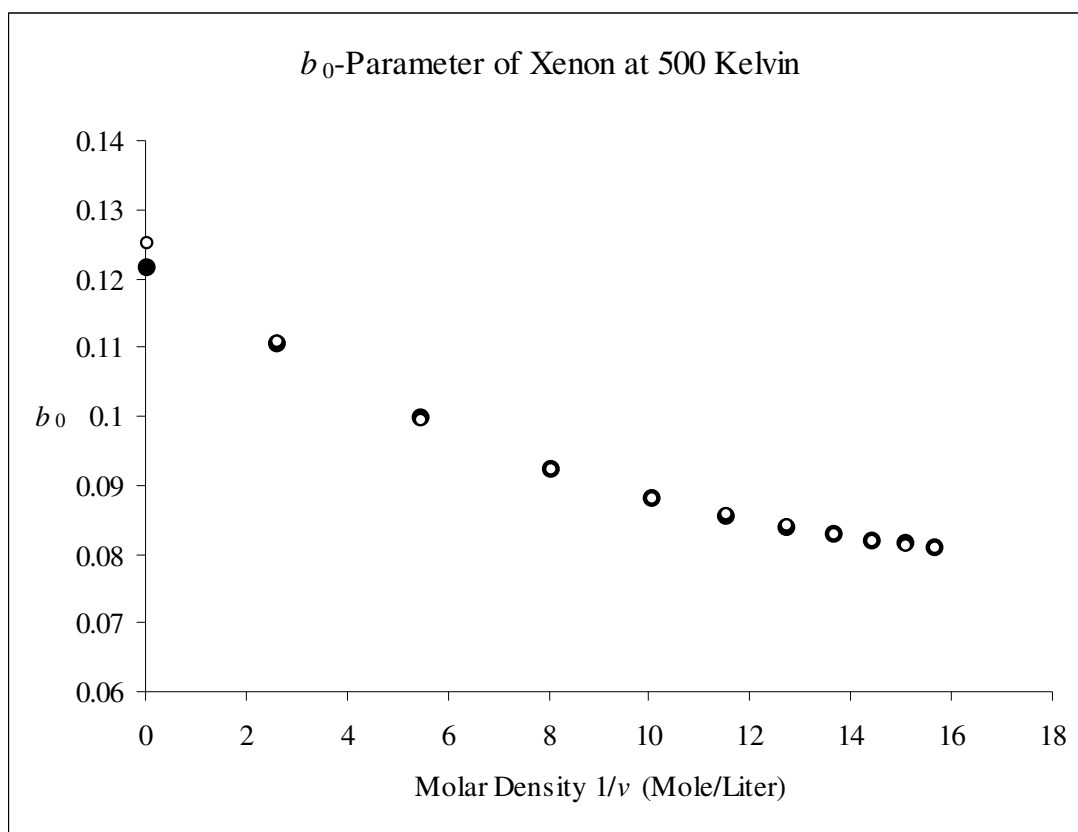


Figure 6 The b_0 -parameter of xenon at 500 Kelvin in units of Liter/mole

The experimental data are represented by the filled-in circles and the fit, utilizing the negative exponential function (Equation 19), are represented by the open circles.

The data point obtained at 1 bar pressure was not used in curve-fitting for the evaluation of the c_0 -, c_1 -, and k_1 -parameters due to increasing experimental error at low molar densities.

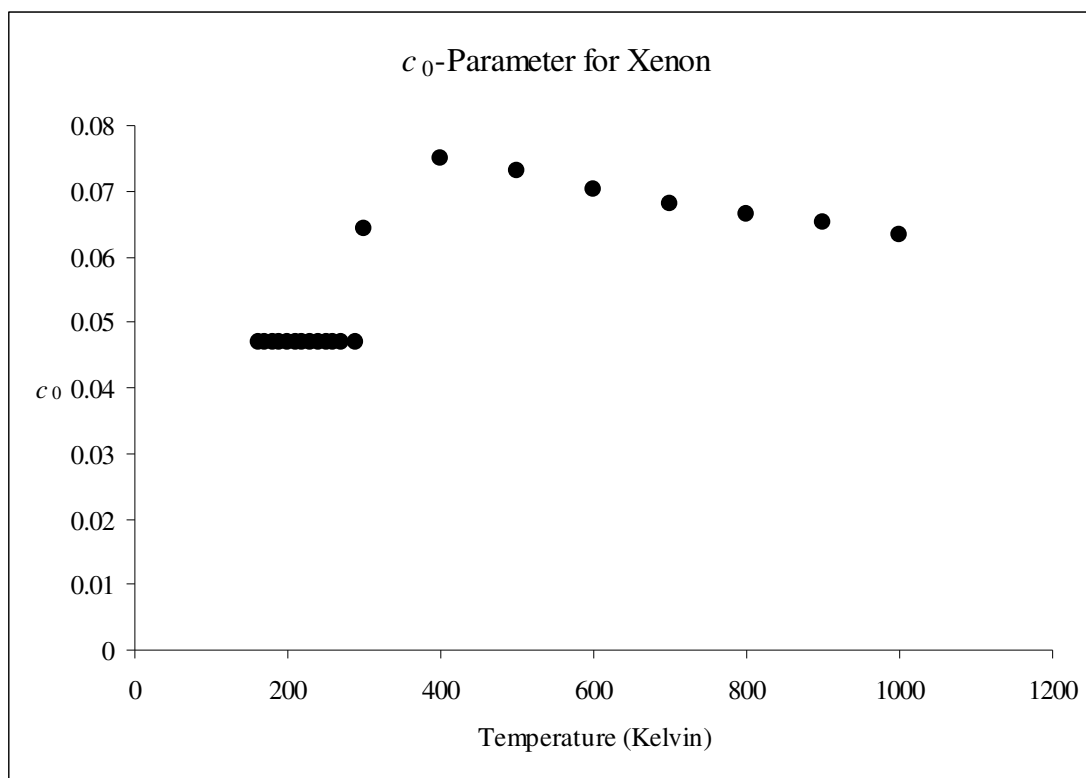


Figure 7 The c_0 -parameter of xenon in units of Liter/mole

At and below the measured critical temperature value of 289.7 Kelvin, the numerical value of the c_0 -parameter is assumed to be constant. This was done mainly for simplification purposes.

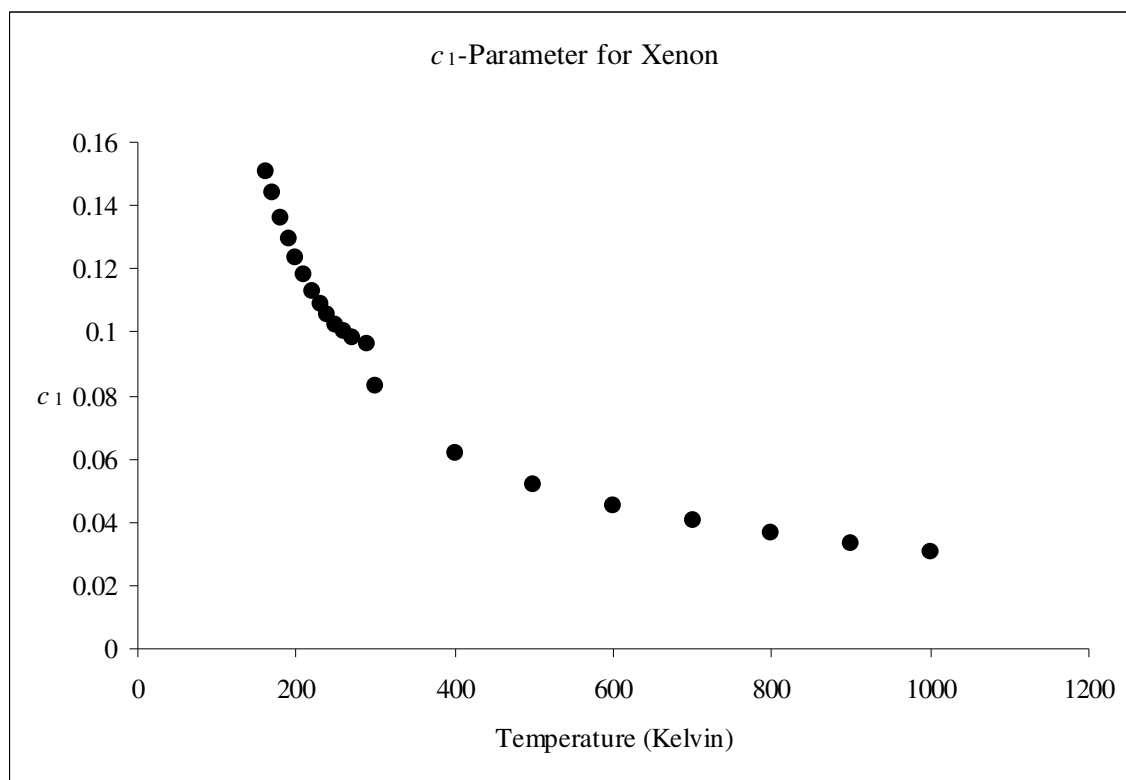


Figure 8 The c_1 -parameter for xenon in units of Liter/mole

Note that discontinuity occurs at the critical temperature value of 289.7 Kelvin

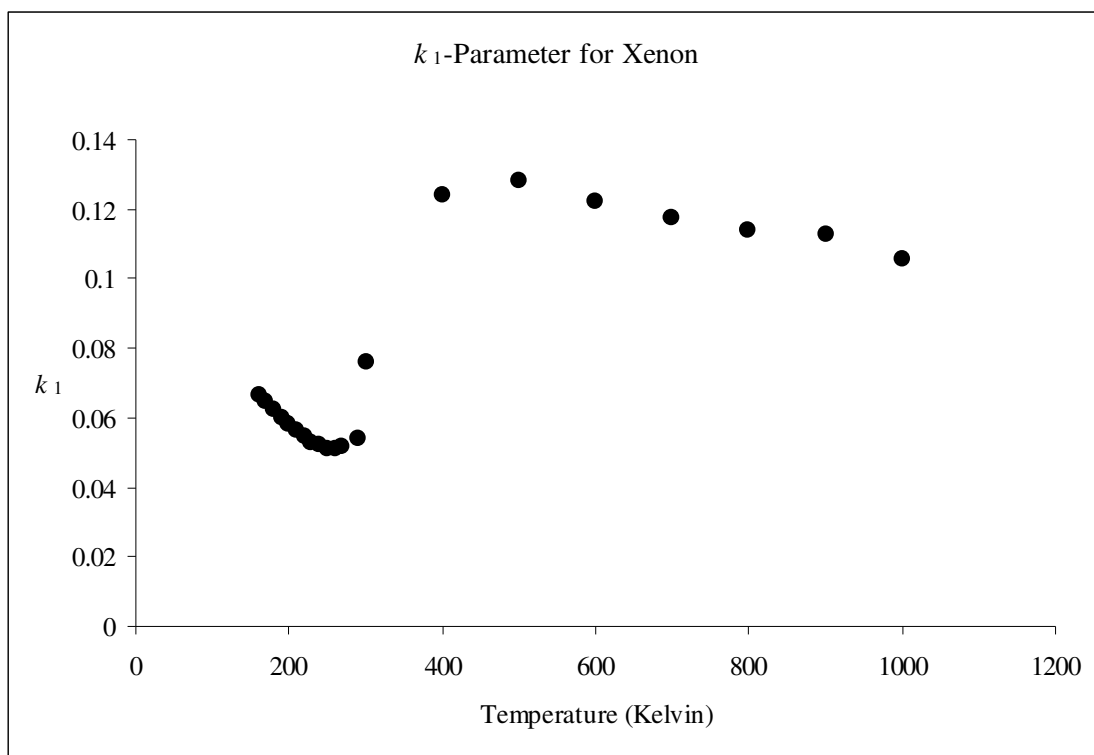


Figure 9 The k_1 -parameter for xenon in units of Liter/mole

Note that discontinuity occurs at the critical temperature value of 289.7 Kelvin

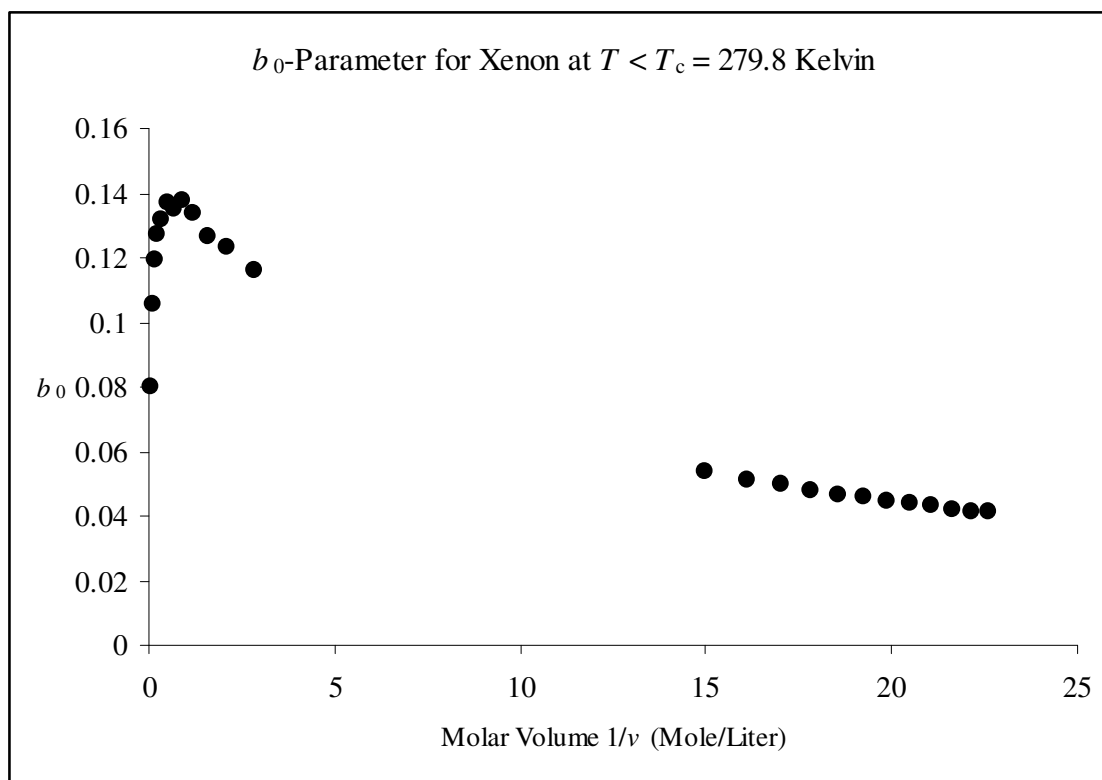


Figure 10 Evaluated b_0 -parameters for xenon, in units of Liter/mole, with the assumption that the f multiplication factor is one ($f = 1$)

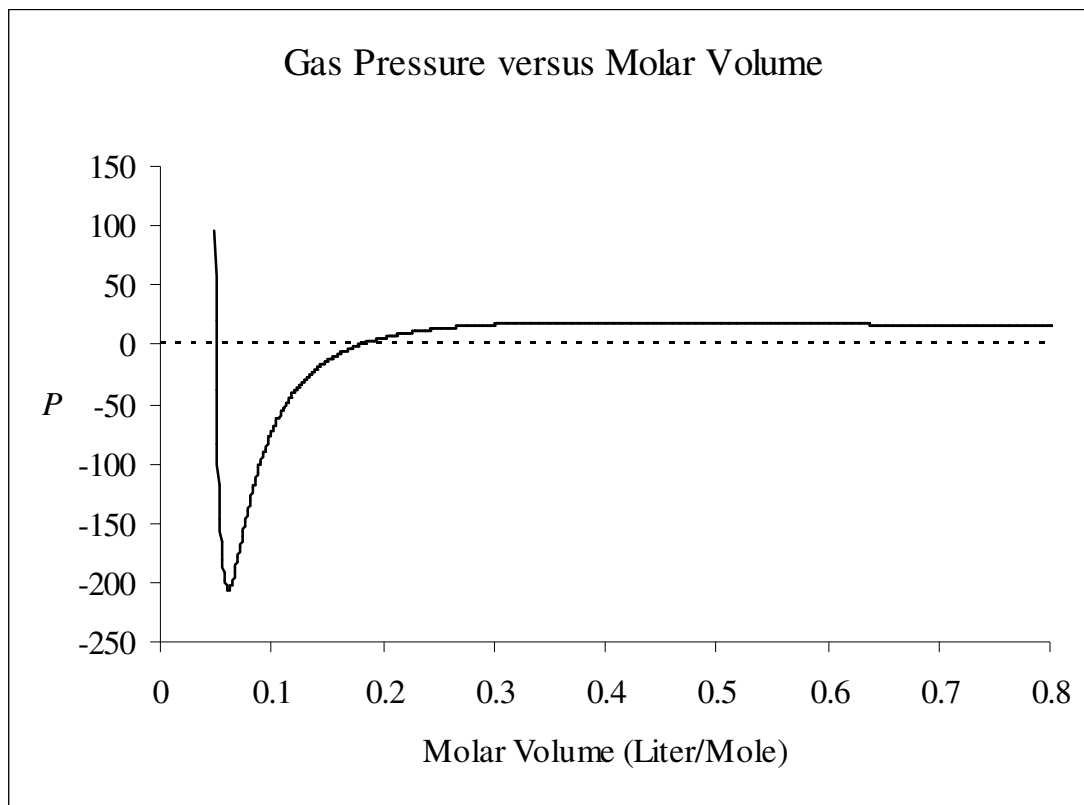


Figure 11 Pressure versus molar volume curve for xenon at temperatures less than the critical temperature value ($T < T_c = 289.7$ Kelvin)

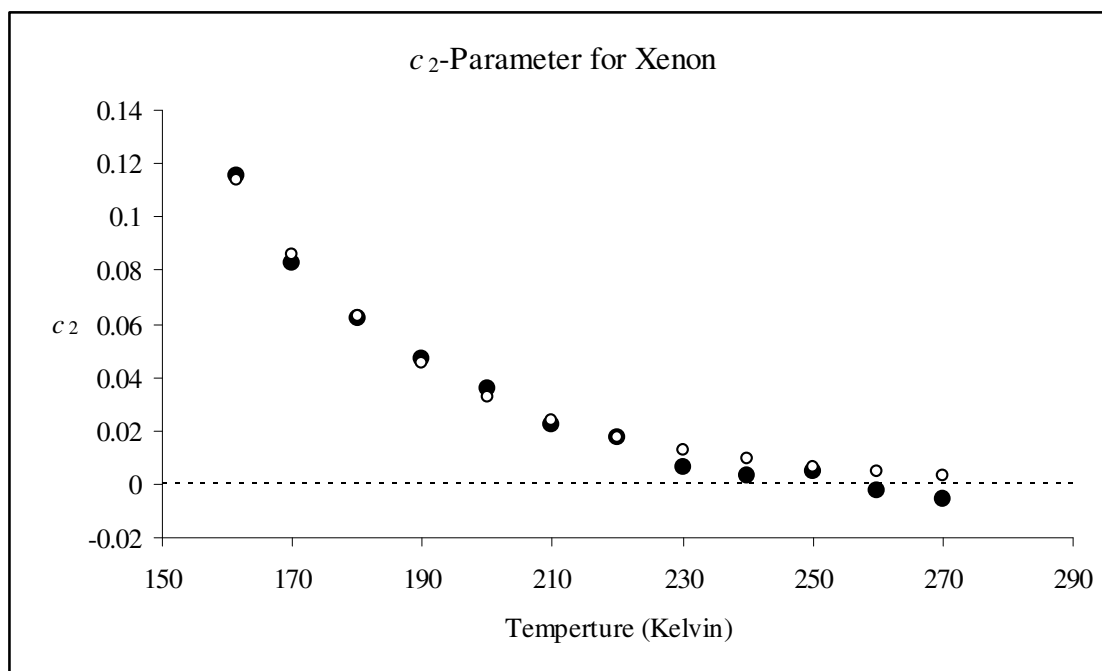


Figure 12 The c_2 -parameter for xenon in units of Liter/mole

Filled-in circles are evaluated data points and the open-circles from the negative exponential fit to the data.

Only the first six data points were used for evaluation of the negative exponential fit.

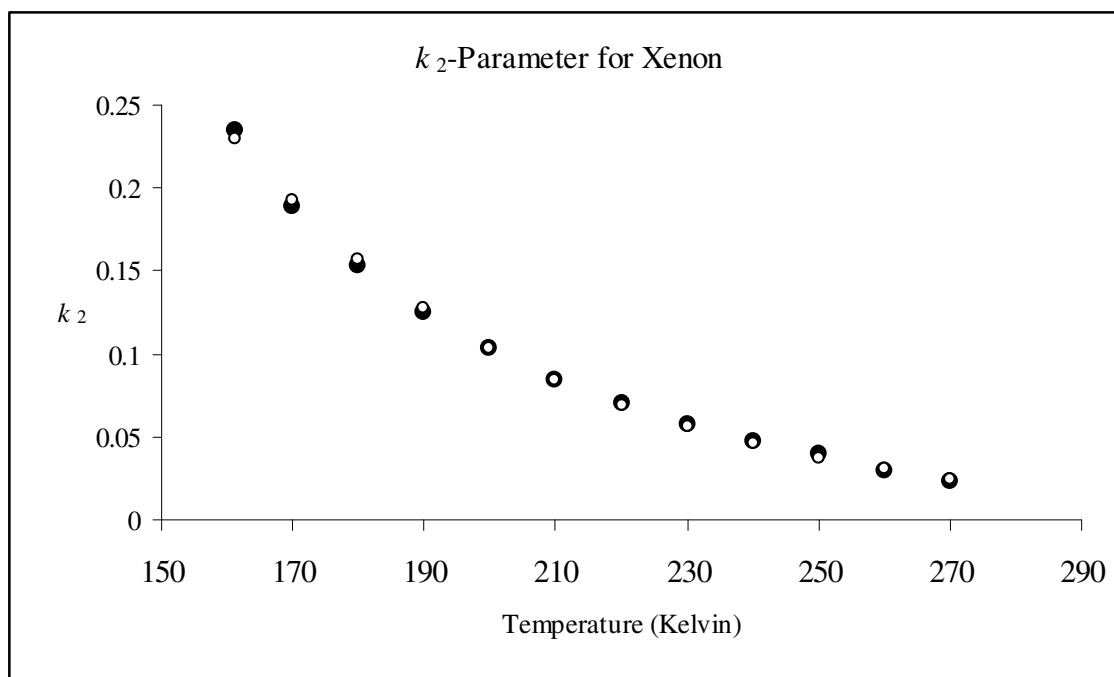


Figure 13 The k_2 -parameter for xenon in units of Liter/mole

Filled-in circles are evaluated data points and the open-circles from the negative exponential fit to the data.

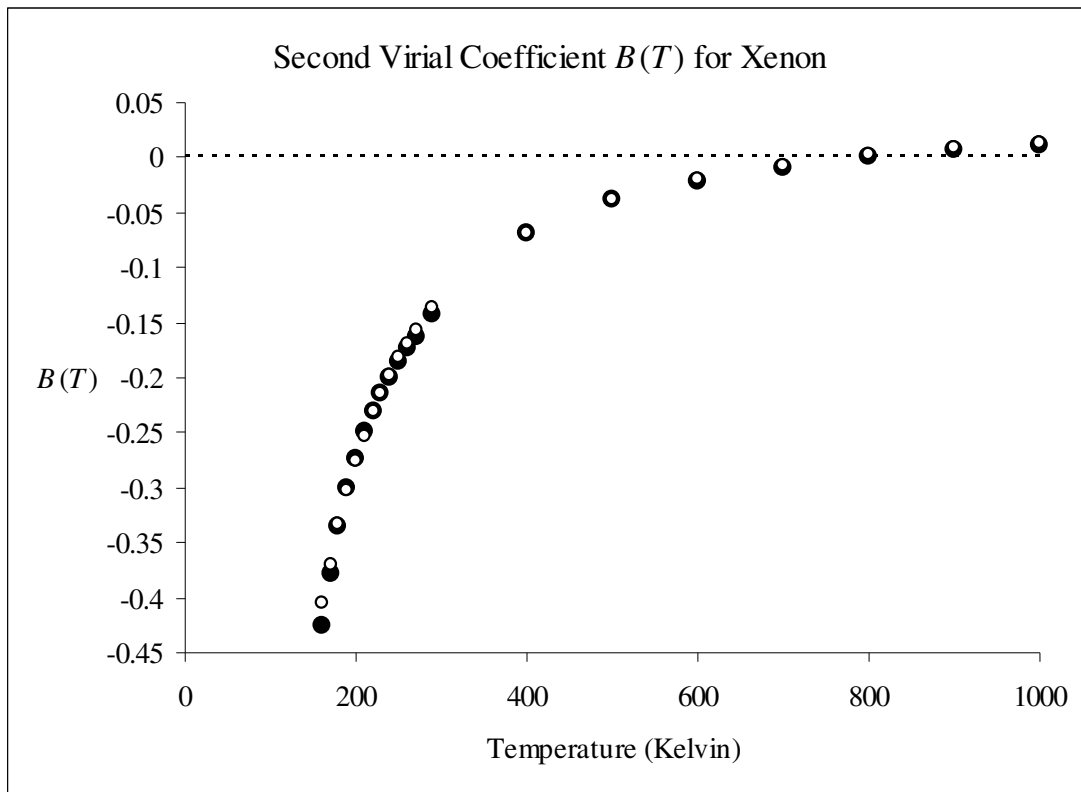


Figure 14 The second virial coefficient for xenon

Filled-in circles are data points obtained for the modified van der Waals expression (Equation 24 incorporating Equations 11, 19, and 25).

Open-circles are from the experimental curve.

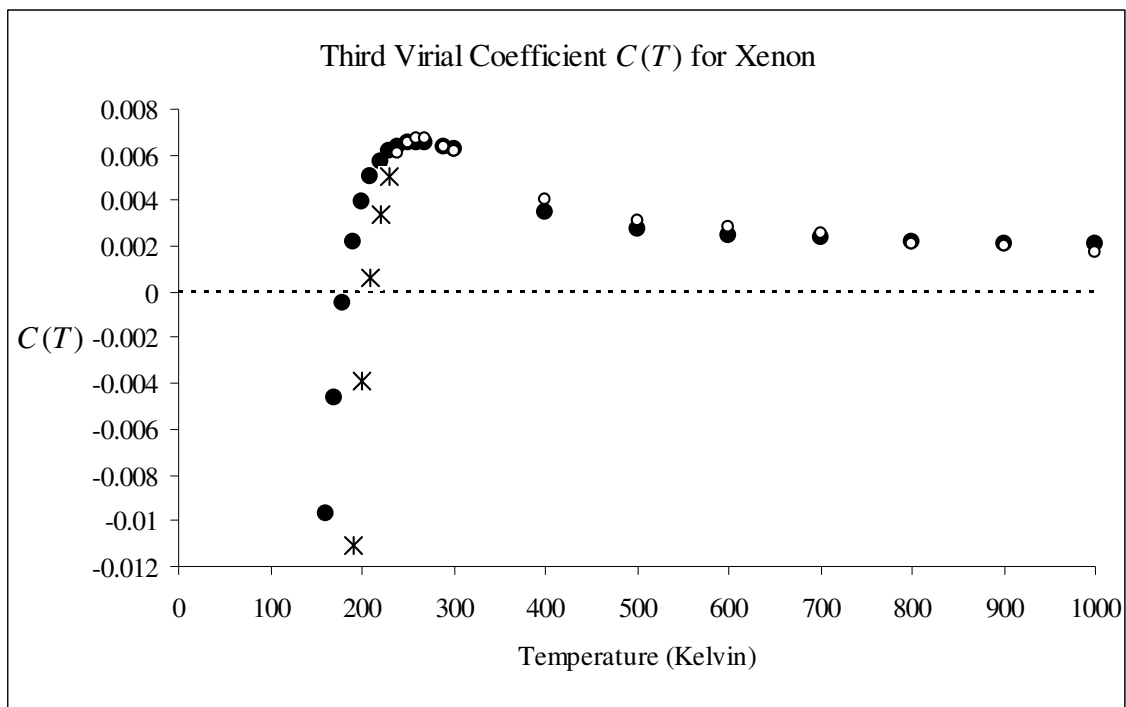


Figure 15 The third virial coefficient for xenon

Filled-in circles are data points obtained for the modified van der Waals expression (Equation 24 incorporating Equations 11, 19, and 25).

Open-circles are from the experimental curve.

Stars are from theoretical calculations. It is nearly impossible to measure the third virial coefficient at low temperatures due to condensation or deposition.

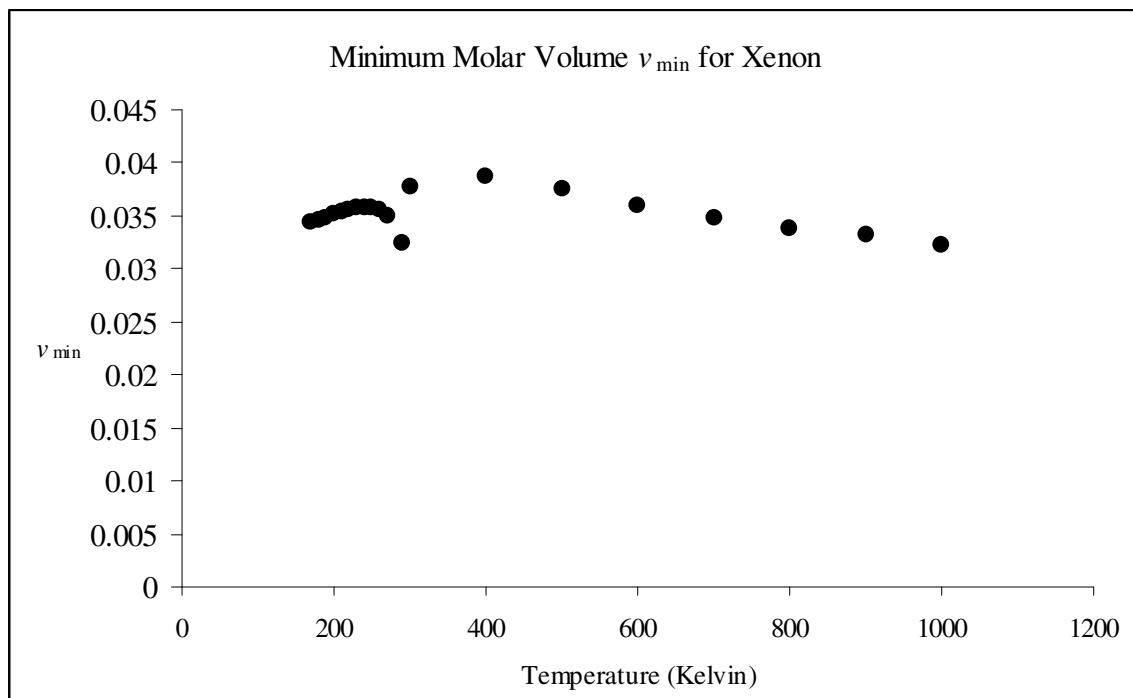


Figure 16 Minimum Molar Volume v_{\min} for Xenon (Liter/Mole)

Minimum molar volume for xenon liquid or gas in the limit of infinite pressures ($P \rightarrow \infty$)

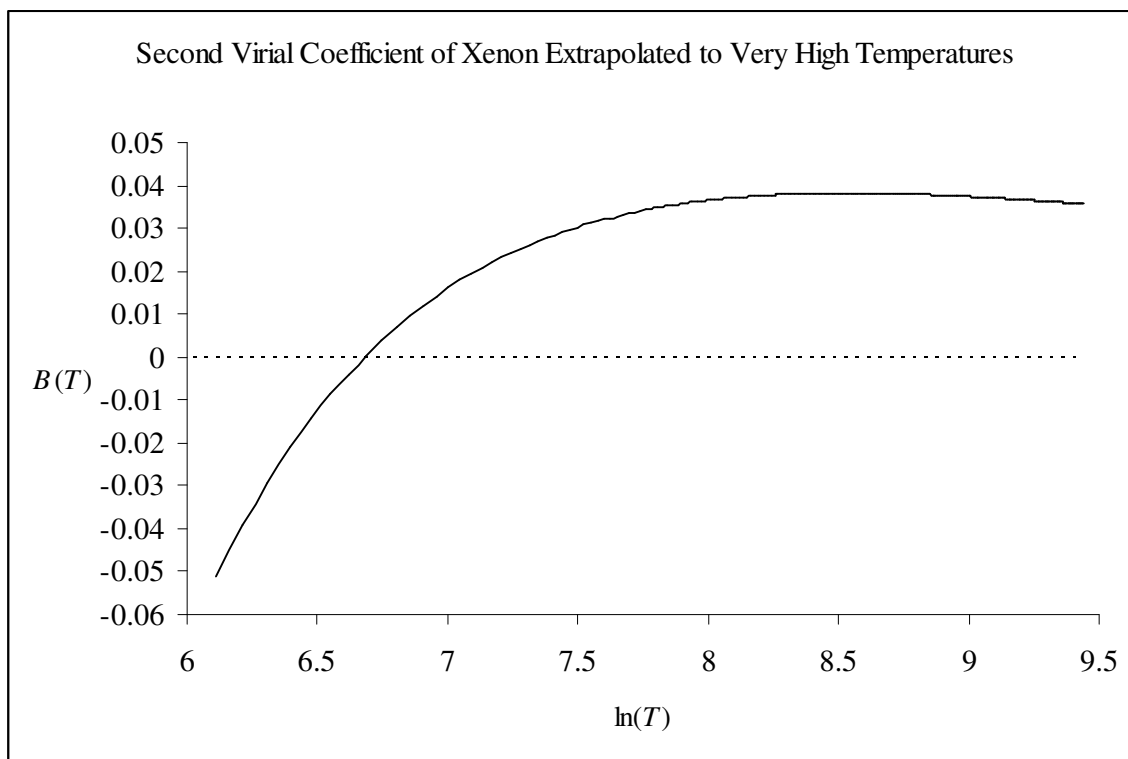


Figure 17 Extrapolated Second Virial Coefficient of Xenon to Extremely High Temperature Values

Maximum in the second virial coefficient occurs around 5,000 Kelvin.

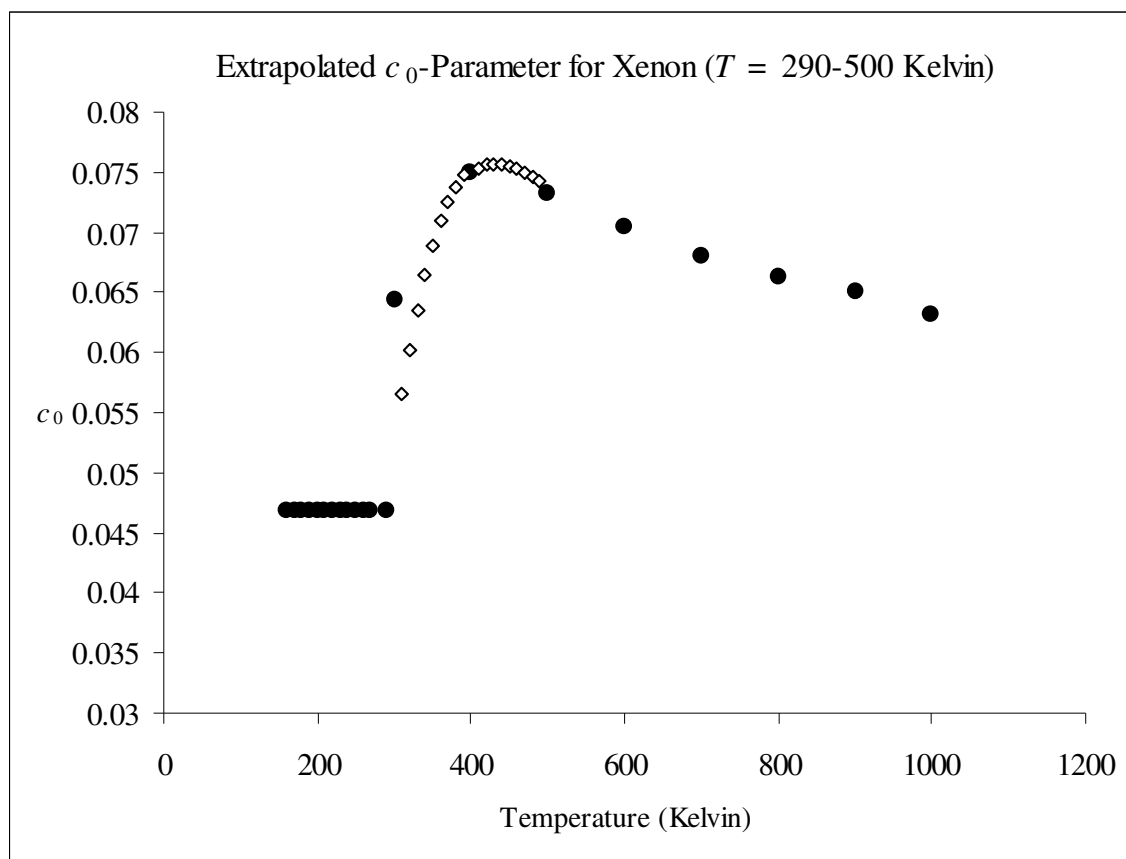


Figure 18 Extrapolated values of the c_0 -Parameter between 290 to 500 Kelvin

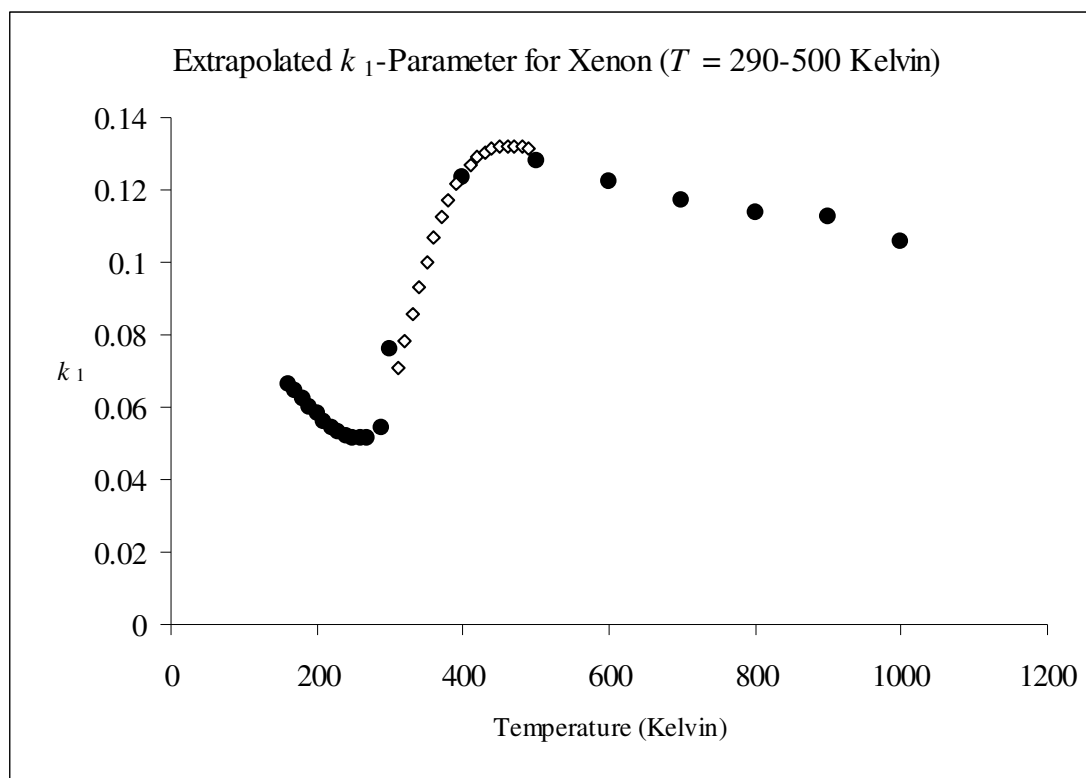


Figure 19 Extrapolated values of the k_1 -Parameter between 290 to 500 Kelvin

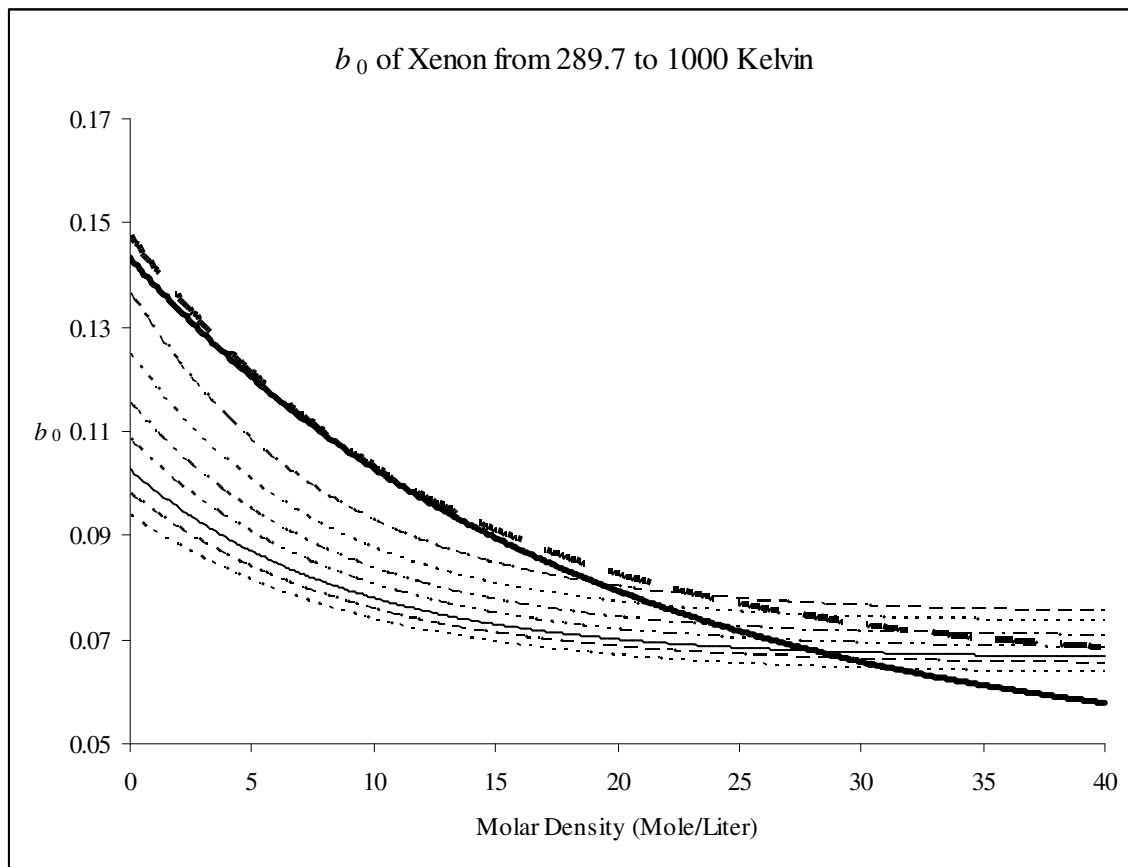


Figure 20 The b_0 -parameter of xenon as a function of the molar density for temperatures above the measured critical temperature value of 289.7 Kelvin

The thick continuous line is at the critical temperature and the thick dashed-line is at 300 Kelvin. The thinner line plots are for 400 to 1000 Kelvin in steps of 100 Kelvin. The lowest thin line plot is for 1000 Kelvin.

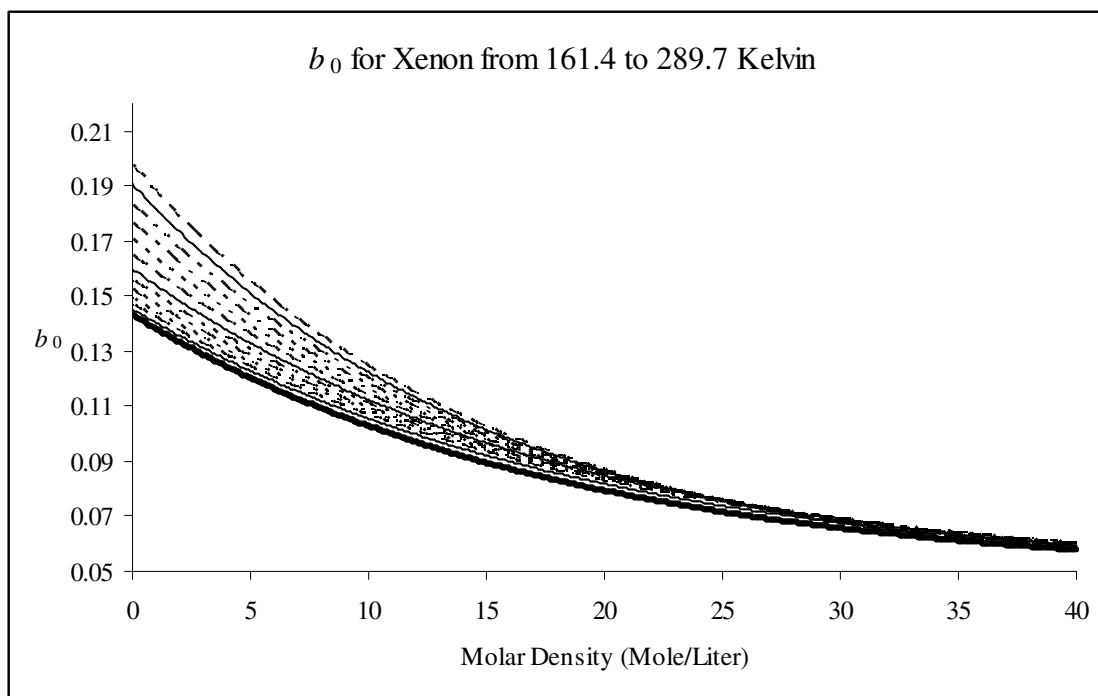


Figure 21 The b_0 -parameter of xenon as a function of the molar density for temperatures below the measured critical temperature value of 289.7 Kelvin

The thick continuous line is at the critical temperature value. The thin lines plotted above the thick line are for temperatures values decreasing from 270 to 170 Kelvin decreasing in steps of 10 Kelvin. The top line is for the melting point of xenon at 161.4 Kelvin.