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Alternative Fuel: Hydrogen and its Thermodynamic Behaviour

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Abstract

Hydrogen is a contender for alternative energy. Hydrogen fuel cell vehicles and hydrogen-based low-carbon fuels will contribute to the decarbonization of the mobility sector, shipping and aviation. Hydrogen is used as a rocket fuel. In addition, petroleum refining, semiconductor manufacturing, aerospace industry, fertilizer production, metal treatment, pharmaceutical, power plant generator, methanol production, commercial fixation of nitrogen from air reduction of metallic ores. Also, hydrogen is used to turn unsaturated fats into saturated fats and oils. In the enhancement of NMR and MRI signals, parahydrogen is used. Parahydrogen and orthohydrogen are nuclear spin isomers of hydrogen. At room temperature, the normal hydrogen at thermal equilibrium consists of 75% orthohydrogen and 25% parahydrogen. The development of hydrogen technology requires knowledge of the thermophysical properties of hydrogen. The second virial coefficient characterizes the primary interaction between the molecules. Therefore, knowledge of the second virial coefficient enables one to determine the pairwise molecular interaction and, in turn, the thermodynamic behaviour of hydrogen. The present study is based on three parameter modified *Berthelot* Equation of state aims to determine the second virial coefficient of hydrogen and its isomers, i.e., orthohydrogen and parahydrogen, over a wide range of temperatures, from the boiling point to the Boyle point. The obtained results are compared with those of the *van der Waals* Equation of state, *Berthelot* Equation of state, *Tsonopoulos* correlation, *McGlashan & Potter* correlation, *Yuan Duan* correlation, *Van Ness & Abbott correlation*, and *McGlashan* correlation. The results of this work agree well with those of other correlations in the high temperature region.

Keywords: Hydrogen; Isomers; Law of Corresponding States; Orthohydrogen; Parahydrogen; Second Virial Coefficient.

1. Introduction

Petroleum refining, semiconductor manufacturing, aerospace industry, fertilizer production, metal treatment, pharmaceutical, power plant generator, methanol production, commercial fixation of nitrogen from air reduction of metallic ores use hydrogen. Hydrogen is a contender for alternative energy. Hydrogen fuel cell vehicles and hydrogen-based low-carbon fuels will contribute to the decarbonization of the mobility sector, shipping and aviation. Hydrogen is used as a rocket fuel, Hydrogen is used to turn unsaturated fats into saturated fats and oils. In NMR and MRI signal enhancement, parahydrogen is employed. The development of hydrogen technology requires knowledge of the thermophysical properties of hydrogen.

Parahydrogen and orthohydrogen are nuclear spin isomers of hydrogen. The nuclear spins of orthohydrogen are parallel and those of parahydrogen are antiparallel. They are chemically identical and have the same atomic and isotopic structure. They differ in the nuclear spin states of their atoms. The energy difference associated with nuclear spin transitions of hydrogen is about 0.1 J.mol^{-1} . However, this tiny change leads to different thermodynamic and spectroscopic properties of hydrogen molecules. The ortho and para hydrogens are characterized by different values of

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specific heat, boiling point, and heat of vaporization. It follows from Pauli's principle that the nuclear spin state and rotational state of the hydrogen molecule are correlated. This is attributed to the fact that the molecules of these gases are rotating differently. Conversion between two nuclear spin states of a hydrogen molecule occurs extremely slowly as the transition between symmetric and antisymmetric nuclear spin states is forbidden by the selection rule of quantum mechanics. Hence, parahydrogen can be stored as an individual gas for longer periods. However, the use of paramagnetic catalysis promotes the establishment of Boltzmann's thermodynamic equilibrium between orthohydrogen and parahydrogen states for a given temperature at an accelerated rate. The paramagnetic materials create a strong inhomogeneous magnetic field at the atomic scale. In such fields, the two hydrogen isomers are no longer equivalent. Hence, the spin-flip transition between orthohydrogen and parahydrogen is no longer forbidden. At room temperature, the normal hydrogen at thermal equilibrium consists of 75% orthohydrogen and 25% parahydrogen. Knowledge about orthohydrogen to parahydrogen conversion is important for the storage of liquid hydrogen. Due to the energy difference associated with different rotational levels, energy is released when orthohydrogen converts to parahydrogen and energy is absorbed in the reverse process.

The scientific and technical significance has led to numerous experimental and theoretical studies on the thermodynamic properties of hydrogen [1-14]. The effect of orthohydrogen and parahydrogen composition on the performance of a proton exchange membrane fuel cell has been calculated and experimentally studied [9]. An equation of state of orthohydrogen and parahydrogen has been derived [10]. The influence of orthohydrogen and parahydrogen conversion is considered to recommend the parameters for hydrogen storage [11]. The sound velocity in liquid parahydrogen, the dielectric constant of liquid parahydrogen along the saturation line, the surface tension of parahydrogen in the temperature range from triple point to critical point, and the density of liquid parahydrogen along the saturation line have been determined [12]. In contrast to bulk metals, the nanoparticles of copper, silver, and gold catalyze the low temperature orthohydrogen to parahydrogen conversion [14].

The present work, based on a modified Berthelot Equation of state, is aimed at determining the second virial coefficient of orthohydrogen and parahydrogen over a wide range of temperature from the boiling point to the Boyle point. The research methodology used in this work is shown in Figure 1.

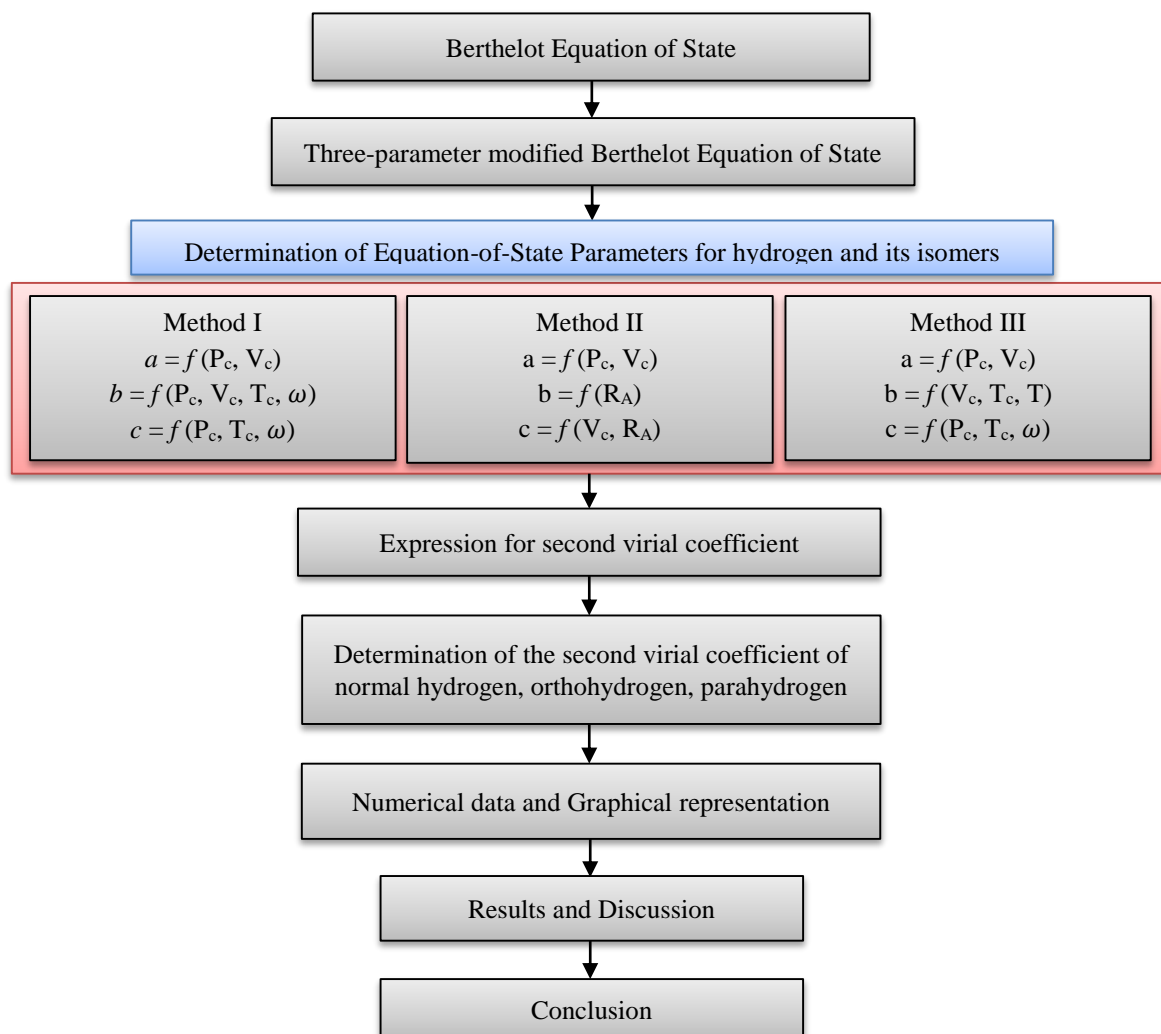


Figure 1. Flowchart of the research methodology

2. Generalized Berthelot Equation-of-State

Many modifications of the known equations of state have been proposed to improve their accuracy [15-22]. The known two – parameter Berthelot equation of state does not quantitatively describe the thermodynamic properties of liquids and gases [23, 24]. With an objective of improving the accuracy, a new parameter is introduced in the repulsive term of the Berthelot equation of state. The modified Berthelot equation of state for one mole of substance is

$$P = \frac{RT}{V-b+c} - \frac{a}{TV^2} \quad (1)$$

The vapour-liquid critical point condition are

$$\left(\frac{\partial P}{\partial V}\right)_{T_c} = 0; \left(\frac{\partial^2 P}{\partial V^2}\right)_{T_c} = 0 \quad (2)$$

where, T_c – Critical temperature.

Applying the conditions given by Equation 2 to Equation 1, the parameters a , b and c in Equation 1 may be determined through the critical - point parameters. Using the obtained expressions for the critical parameters, Equation 1 rewritten in the reduced form as:

$$P^* = \frac{8T^*}{3V^*-1} - \frac{3}{T^*V^{*2}} \quad (3)$$

where, $P^* = P/P_c$, $V^* = V/V_c$, $T^* = T/T_c$, P_c - Critical pressure, V_c – Critical volume. The reduced equation of state given by Equation 3 represents the two-parameter law of corresponding states.

Method – I

The parameter a is determined using critical-point, parameters by:

$$a = \frac{8 P_c^2 V_c^3}{R} \quad (4)$$

The substance-specific parameter c is calculated through the Peneloux correlation [25] by:

$$c = 0.40768 (0.29441 - Z_{RA}) \frac{RT_c}{P_c} \quad (5)$$

where, Z_{RA} - Rackett compressibility factor.

$$Z_{RA} = (0.29056 - 0.08775)\omega$$

where, ω - Pitzer's acentric factor.

The parameter b is determined using the critical volume and the parameter c by:

$$b_c = \frac{V_c + 3c}{3} \quad (6)$$

Method – II

The parameter a calculated by Equation 4 as in the Method – I. The parameter b is determined through the atomic radius by the relation [26] by:

$$b = \frac{16\pi}{3} R_A^3 N_A \quad (7)$$

where, N_A – Avagadro's Number, R_A – Atomic radius.

The parameter c is determined using the critical volume and the parameter b determined by Equation 7. That is;

$$c = \frac{3b - V_c}{3} \quad (8)$$

Method – III

In this method, b is considered to be temperature dependent. The parameters a and c are calculated through Equations 4 and 5 as in Method-I. The parameter b is determined using critical volume as:

$$b_c = \frac{V_c + 3c}{3} \quad (9)$$

The temperature dependence of the covolume b is given [27] by:

$$b(T) = b_c \left(\frac{T_c}{T}\right)^{\frac{1}{3}} \quad (10)$$

3. Determination of the Equation-of-State-Parameters

Using Equations 4 to 10, the parameters a , b and c of the generalized Berthelot equation of state are determined through data [28] on the vapor – liquid critical parameters for hydrogen and its isomers. The obtained values of the parameters a , b and c are presented in Tables 1 and 2.

Table 1. Equation-of-state parameters by Methods – I, and II

Substance	Method – I			Method – II		
	$a \times 10^3$ Pa ² m ⁹ K/mol ⁴ /J	$b \times 10^5$ m ³ /mol	$c \times 10^5$ m ³ /mol	$a \times 10^3$ Pa ² m ⁹ K/mol ⁴ /J	$b \times 10^5$ m ³ /mol	$c \times 10^5$ m ³ /mol
Normal Hydrogen	427.8286	2.0057	-0.1343	427.8286	1.7428	-0.3972
Orthohydrogen	442.9450	2.0197	-0.1293	442.9450	1.7428	-0.4062
Parahydrogen	424.1882	2.0132	-0.1321	424.1882	1.7428	-0.4025

Table 2. Equation-of-state parameters by Method – III

Substance	$a \times 10^3$ Pa ² m ⁹ K/mol ⁴ /J	$c \times 10^5$ m ³ /mol	$b(T) \times 10^5$ m ³ /mol						
			20K	25K	30K	35K	40K	45K	50K
Normal hydrogen	427.8286	-0.1343	2.4821	2.3041	2.1683	2.0597	1.9700	1.8942	1.8288
Orthohydrogen	442.9450	-0.1293	2.4902	2.3117	2.1754	2.0665	1.9765	1.9004	1.8348
Parahydrogen	424.1882	-0.1321	2.4821	2.3042	2.1683	2.0597	1.9700	1.8942	1.8288

4. Second Virial Coefficient by the Modified Berthelot Equation of State

The compressibility factor may be expressed [29] in terms of a series in $1/V$ to get the virial equation of state as:

$$Z = \frac{PV}{RT} = 1 + \frac{B_2}{V} + \frac{B_3}{V^2} \dots \quad (11)$$

where, B_2 -second virial coefficient, B_3 – third virial coefficient and so on.

For a given substance, the virial coefficient depends only on temperature. The second virial coefficient is a measure of pair-wise intermolecular interaction. And, the third virial coefficient is a measure of intermolecular interaction between three molecules. Hence, the knowledge of the virial coefficient will enable one to determine the intermolecular potential of substances. In general, reliable data on the virial coefficient of substances are scarce.

The second virial coefficient is given [30] by:

$$B_2 = \left(\frac{\partial Z}{\partial \rho} \right)_T \quad \text{at} \quad \rho = 0 \quad (12)$$

where, Z – Compressibility factor, ρ - molar density.

For fluids obeying Equation 1, the compressibility factor is given by:

$$Z = \frac{1}{1-(b-c)\rho} - \frac{a\rho}{RT^2} \quad (13)$$

From Equations 12 and 13, we get the second virial coefficient correlated to the equation-of-state parameters as:

$$B_2 = b - c - \frac{a}{RT^2} \quad (14)$$

5. Second Virial Coefficient of Hydrogen and its Isomers

The second virial coefficients of normal hydrogen, orthohydrogen, parahydrogen at various temperatures are determined by Equation 14 with the values of the parameters a , b and c presented in Tables 1 and 2. The obtained values of the second virial coefficients for normal hydrogen, orthohydrogen, parahydrogen are presented in Tables 3 to 5. For comparison, the second virial coefficient of hydrogen and its isomers has been determined by the Berthelot Equation of state [31], van der Waals Equation of state [32], Van Ness & Abbott correlation [33], Yuan Duan correlation [34], McGlashan & Potter correlation [35], McGlashan correlation [36], and Tsonopoulos correlation [37]. The results are also presented in Tables 3 to 5. The temperature dependence of the second virial coefficient of hydrogen and its isomers is depicted in Figures 1 to 3.

Table 3. Second virial coefficient of Normal Hydrogen

<i>T</i> (K)	$B_2 \times 10^{-5} \text{ (m}^3\text{.mol}^{-1}\text{)}$									
	Equation 14			vdW EoS	McG	Tsono	Berth EoS	McGP	YD	VNA
	Method-I	Method-II	Method-III							
20	-10.3953	-10.7239	-10.8526	-7.5047	-18.8165	-11.8810	-0.2610	-0.1450	-7.0167	-12.3468
25	-6.0934	-6.0929	-5.8016	-5.5753	-12.2652	-10.2494	0.6034	-0.0790	-7.4807	-10.4060
30	-3.5829	-3.5773	-3.4196	-4.2894	-8.6717	-8.1404	1.1028	-0.0468	-7.1808	-8.2421
35	-2.0607	-2.0604	-2.0998	-3.3709	-6.4270	-6.4699	1.3560	-0.0291	-6.7141	-6.5156
40	-0.9919	-1.10759	-1.1144	-2.6860	-4.8981	-5.1774	1.5397	-0.0196	-6.2125	-5.2005
45	-0.4010	-0.4010	-0.5147	-2.1463	-3.7952	-4.1750	1.6658	-0.0143	-5.7134	-4.1980
50	0.0796	-0.0969	-0.0969	-1.7177	-2.9620	-3.9049	1.7558	-0.0093	-5.2288	-3.4174

Table 4. Second virial coefficient of Orthohydrogen

<i>T</i> (K)	$B_2 \times 10^{-5} \text{ (m}^3\text{.mol}^{-1}\text{)}$									
	Equation 14			vdW EoS	McG	Tsono	Berth EoS	McGP	YD	VNA
	Method-I	Method-II	Method-III							
20	-10.653	-11.1702	-10.6805	-7.6814	-18.3198	-11.8260	-0.2451	-0.9983	-6.9519	-16.7141
25	-6.3753	-6.3748	-6.0710	-5.7153	-11.9449	-10.0249	0.6226	-0.0782	-7.3646	-10.1861
30	-3.7706	-3.7706	-3.6064	-4.4046	-8.4451	-7.9531	1.0799	-0.0463	-7.0547	-6.3545
35	-2.2004	-2.1998	-2.1471	-3.4683	-6.2562	-6.3115	1.3706	-0.0293	-6.5880	-8.0499
40	-1.0948	-1.1808	-1.2192	-2.7662	-4.7658	-5.0486	1.5437	-0.0104	-6.0899	-5.0687
45	-0.4819	-0.4818	-0.5974	-2.2200	-3.6889	-4.0654	1.6778	-0.0132	-5.5957	-4.0853
50	0.0180	0.0179	-0.1639	-1.7831	-2.8759	-3.2856	1.7673	-0.0091	-5.1160	-3.3241

Table 5. Second virial coefficient of Parahydrogen

<i>T</i> (K)	$B_2 \times 10^{-5} \text{ (m}^3\text{.mol}^{-1}\text{)}$									
	Equation 14			vdW EoS	McG	Tsono	Berth EoS	McGP	YD	VNA
	Method-I	Method-II	Method-III							
20	-10.1276	-10.6099	-10.1408	-7.4648	-18.4570	-11.9989	-0.2937	-0.1303	-7.0806	-12.3230
25	-6.018	-6.0198	-5.7269	-5.5427	-12.0368	-10.1338	0.5877	-0.0776	-7.4751	-10.387
30	-3.5236	-3.5236	-3.3685	-4.2614	-8.5095	-8.0300	1.0583	-0.0459	-7.1527	-8.1277
35	-2.0196	-2.0217	-1.9731	-3.3461	-6.3021	-6.3678	1.3506	-0.0290	-6.6753	-6.4628
40	-0.9566	-1.0435	-1.0866	-2.6597	-5.1078	-5.0903	1.5315	-0.0157	-6.1673	-5.1101
45	-0.3742	-0.3764	-0.4932	-2.1258	-3.7118	-4.0961	1.6645	-0.0131	-5.6639	-4.1524
50	0.0179	0.1044	-0.0799	-1.6987	-2.8912	-3.3078	1.7558	-0.0090	-5.1754	-3.3499

where vdW Eos- van der Waals Equation of State, McG - McGlashan Correlation, Tsono - Tsonopoulos Correlation, Berth Eos- Berthelot Equation of State, McGP - McGlashan and potter Correlation, YD - Yuan Duan Correlation, VNA - Van Ness Abbott Correlation.

The equation-of-state parameters a , b , and c for normal hydrogen, orthohydrogen, and parahydrogen have been calculated using three different methods. In all three methods, the parameter a is determined through the critical pressure and critical volume of normal hydrogen, orthohydrogen, parahydrogen. This is justified by the fact that in the known Berthelot equation of state, only the repulsive term has been modified in this work. To investigate its impact on the performance of the given equation of state, the parameter b is determined by three different ways and the parameter c is determined by two different methods. The values of the parameter b for normal hydrogen, orthohydrogen and parahydrogen calculated through the critical-point parameters and through the atomic radius differ by a factor of about 3. In these two methods, the parameter b is considered to be temperature independent. In the third method, a temperature dependence of the parameter b is considered. The values of the parameter c for normal hydrogen, orthohydrogen, parahydrogen are determined in two different ways. One through the critical-point parameters and the acentric factor and another through the critical volume and the atomic radius. The obtained values of parameter c differ by a factor of about 1.6.

Having obtained the values of the parameters a , b , and c , the second virial coefficient of normal hydrogen, orthohydrogen, and parahydrogen is calculated over a wide temperature range. As seen from Tables 3 to 5 and Figures 2 to 4, the three methods yield approximately the same value of the second virial coefficient at a certain temperature

for a studied substance. As seen from Tables 3 to 5, the input data used for the determination of the covolume b of normal, ortho, and parahydrogen do not have a substantial impact. When compared to the McGlashan correlation, Van Ness & Abbott correlation, Tsonopoulos correlation, van der Waals equation of state, and Yuan Duan correlation, the modified Berthelot equation of state gives higher values for the second virial coefficient of normal hydrogen, orthohydrogen, and parahydrogen, and it gives smaller values when compared to the Berthelot equation of state and McGlashan & Potter correlation. This discrepancy substantially decreases in the high-temperature zone. Moreover, the modified Berthelot equation of state proposed in this work and the McGlashan correlation reveal the typical trend of temperature dependence of the second virial coefficient of substances below the Boyle temperature. Berthelot and McGlashan & Potter give the unphysical values (positive values) of the second virial coefficient for normal hydrogen, orthohydrogen, and parahydrogen at temperatures exceeding 20K.

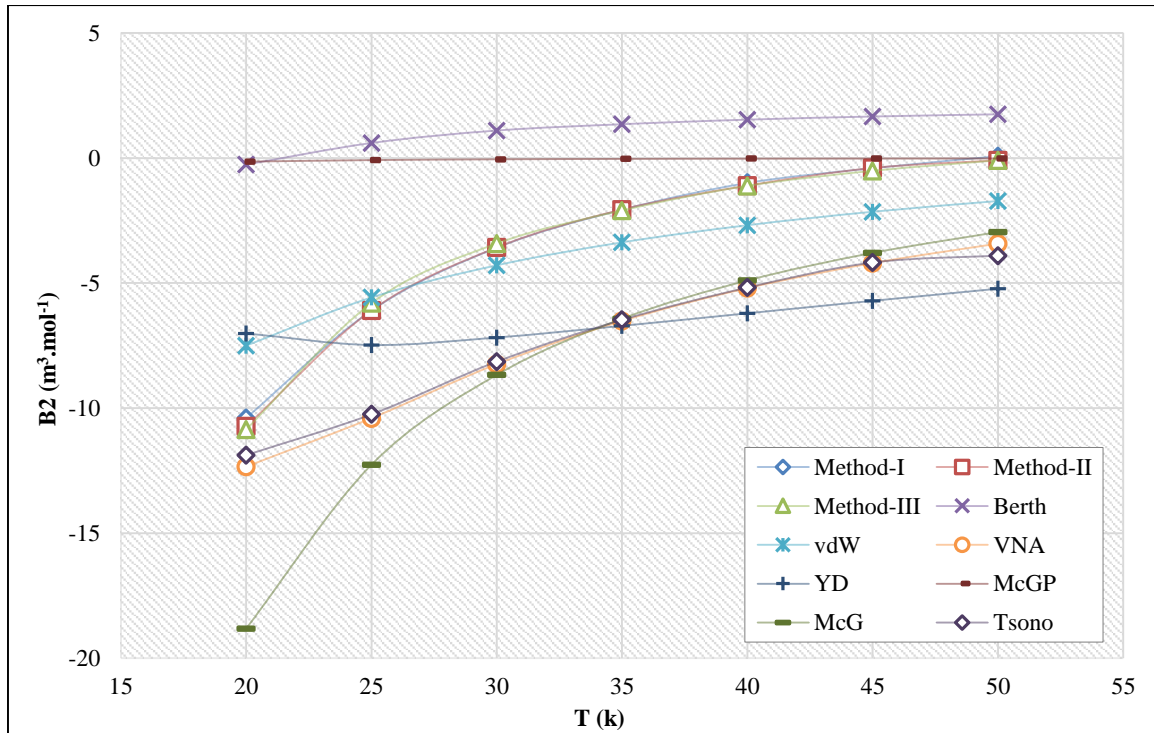


Figure 2. Second Virial Coefficient of Normal Hydrogen

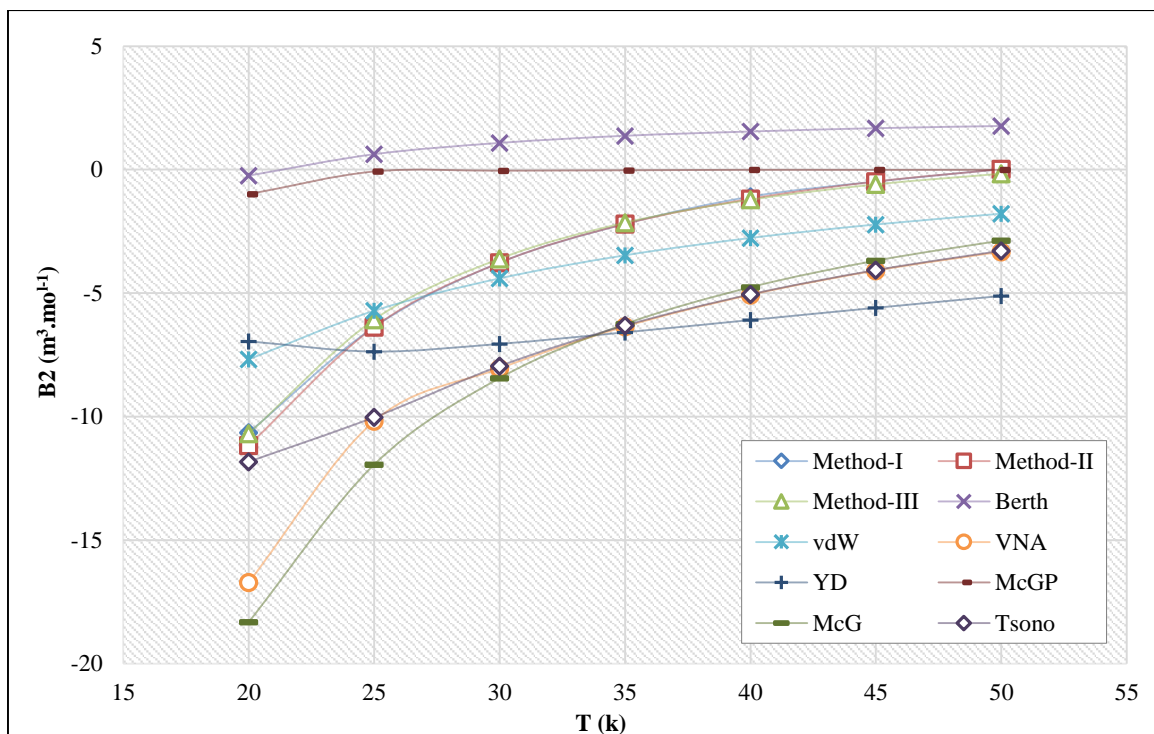


Figure 3. Second Virial Coefficient of Orthohydrogen

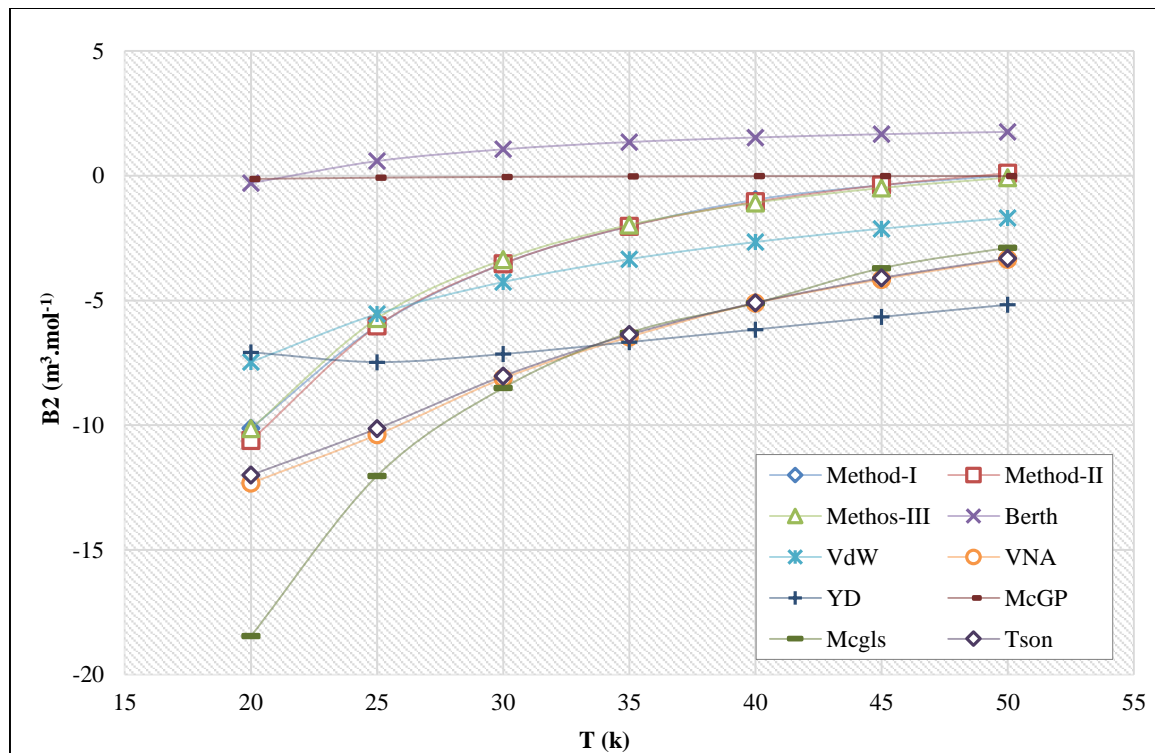


Figure 4. Second Virial Coefficient of Parahydrogen

6. Conclusion

A modified Berthelot equation of state with three substance-specific parameters a , b , and c has been employed to determine the second virial coefficient of normal hydrogen, orthohydrogen, and parahydrogen in a wide range of temperatures up to the vicinity of the vapour-liquid critical point and beyond. Three different methods have been used to calculate the equation-of-state parameters a , b , and c for normal hydrogen, orthohydrogen, and parahydrogen. The three methods yield approximately the same value of the second virial coefficient at a certain temperature for a studied substance. The input data used for the covolume of normal, ortho, and parahydrogen does not have a substantial impact. The modified Berthelot equation of state for the second virial coefficient of normal hydrogen, orthohydrogen and parahydrogen gives higher values compared to the McGlashan correlation, Van Ness & Abbott correlation, Tsonopoulos correlation, van der Waals Equation of state, and Yuan Duan correlation, while it gives smaller values of second virial coefficient compared to the Berthelot equation of state, McGlashan & Potter correlation. In the high-temperature region, this discrepancy greatly decreases.

7. Declarations

7.1. Author Contributions

Conceptualization, R.B.; methodology, R.B.; software, A.A.; validation, S.G.; formal analysis, R.B.; investigation, S.G.; data curation, K.J.; writing—original draft preparation, R.B.; writing—review and editing, R.B. All authors have read and agreed to the published version of the manuscript.

7.2. Data Availability Statement

The data presented in this study are available on request from the corresponding author.

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The authors received no financial support for the research, authorship, and/or publication of this article.

7.4. Institutional Review Board Statement

Not applicable.

7.5. Informed Consent Statement

Not applicable.

7.6. Declaration of Competing Interest

The authors declare that there is no conflict of interests regarding the publication of this manuscript. In addition, the ethical issues, including plagiarism, informed consent, misconduct, data fabrication and/or falsification, double publication and/or submission, and redundancies have been completely observed by the authors.

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