



Thermodynamic Properties and Phase Equilibria for Liquid Fluorine Using GMA Equation of State

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Abstract

Thermophysical properties of fluorine are interesting because of its applications in different areas of technology and industry. The computations of thermodynamic properties were performed with the GMA equation of state under critical conditions. The present work reports calculations of density, volumetric, and thermodynamic properties of liquid fluorine on extended ranges of pressure and temperature and the results show that GMA equation of state reproduces the experimental *PVT* data of fluorine within experimental errors throughout the liquid phase. The calculated results are different only a few percent from the experimental ones.

Keywords: GMA Equation of state, liquid fluorine, speed of sound, *VLE* prediction

1. Introduction

Fluorine is one of the most powerful oxidizing agent known and reacting with practically all organic and inorganic substances. Because of its very high reactivity, fluorine has a universal application as a fluorinating agent. In dense concentrations and in the liquid state it has a pale greenish yellow color. It has characteristic odor, similar to a mixture of ozone and chlorine. Fluorine is so toxic and reactive that its physical properties are difficult to measure [1].

In the course of study of the thermodynamic properties of gaseous and liquid fluorine, Straty and Prydz, at 1970, measured the melting pressures of fluorine from the triple point to a maximum pressure of 9.869 atm [2]. In addition, Kanda has measured *PVT* properties of fluorine [3].

Fluorine has widespread applications in

modern industry and technology; therefore, existence of an equation of state for prediction of the physical and chemical properties of this material is necessary. Some equations of state have been used to calculate thermodynamic properties of fluorine [4-9].

Equations of state are required for the calculations of thermodynamic properties needed in process engineering. For the development of accurate equations of state, a large amount of high-quality thermodynamic data is essential. Information about the pressure and temperature dependencies of such properties allows for thermodynamic modeling based on equations of state, statistical mechanics, and so forth to be checked. Among these properties, density values as a function of temperature and pressure are needed for the development of correlation or prediction models [10].

The goal of the present study is to investigate the results of simultaneous calculations of *PVT* data, thermodynamic properties such as

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isobaric expansion coefficient, α , isothermal compressibility, κ , speed of sound, w , Joule-Thomson coefficient, μ_{JT} , and vapor-liquid equilibrium, VLE prediction, for fluorine by using GMA equation of state (proposed by Goharshadi-Morsali-Abbaspour) [11,12].

A wide comparison with literature experimental data was made. The accuracy of the equation of state was determined by the absolute average deviation statistical parameter (AAD).

2. Theoretical Basis

Equation of state is a fundamental characteristic of matter defining its thermodynamic properties in a wide range of pressure and temperature. Knowledge of the thermodynamic properties of materials is required for numerous fundamental and applied problems. Recently, GMA equation of state has been developed that is applicable to liquids in the subcritical region, namely, $T < T_c$ (and $\rho > \rho_c$) [11] where T and ρ are temperature and density, respectively.

The GMA equation of state [11] for liquid state is in the form:

$$(2Z - 1)V_m^3 = A(T) + B(T)\rho \quad (1)$$

where Z is the compression factor, V_m is the molar volume, ρ is the density ($\rho = 1/V_m$), and $A(T)$ and $B(T)$ parameters depend on temperature via the equations:

$$A(T) = A_o - \frac{2A_1}{RT} + \frac{2A_2 \ln T}{R} \quad (2)$$

and

$$B(T) = B_o - \frac{2B_1}{RT} + \frac{2B_2 \ln T}{R} \quad (3)$$

here, A_o , A_1 , A_2 , B_o , B_1 , and B_2 are parameters and R is the universal gas constant.

The GMA equation of state has been applied to liquid densities calculations of different pure and mixture fluids including polar, nonpolar, and hydrogen bonded liquids [11-15].

Using this equation of state, we have derived thermodynamic quantities of fluorine and compared them with experiment [16].

3. Results and Discussion

Using GMA equation of state, A_o to A_2 and B_o to B_2 constants has been computed for liquid fluorine. The constants of equation of state for fluorine are:

$$\begin{aligned} A_o &= 3.74397 \times 10^{-3} \text{ (L}^3 \text{ mol}^{-3}\text{)} \\ B_o &= -6.19735 \times 10^{-5} \text{ (L}^4 \text{ mol}^{-4}\text{)} \\ A_1 &= 6.82738 \times 10^{-3} \text{ (L}^4 \text{ atm mol}^{-4}\text{)} \\ B_1 &= -1.31855 \times 10^{-4} \text{ (L}^5 \text{ atm mol}^{-5}\text{)} \\ A_2 &= -2.31905 \times 10^{-5} \text{ (L}^4 \text{ atm mol}^{-4} \text{ K}^{-1}\text{)} \\ B_2 &= 3.88678 \times 10^{-7} \text{ (L}^5 \text{ atm mol}^{-5} \text{ K}^{-1}\text{)} \end{aligned}$$

3.1. Density

The isotherms of $(2Z - 1)V_m^3$ are linear functions of density with slope $B(T)$ and intercept $A(T)$ (GMA equation of state), Fig. 1 indicates the isotherms of liquid fluorine. The constants of equation of state were computed by using the slope and intercept.

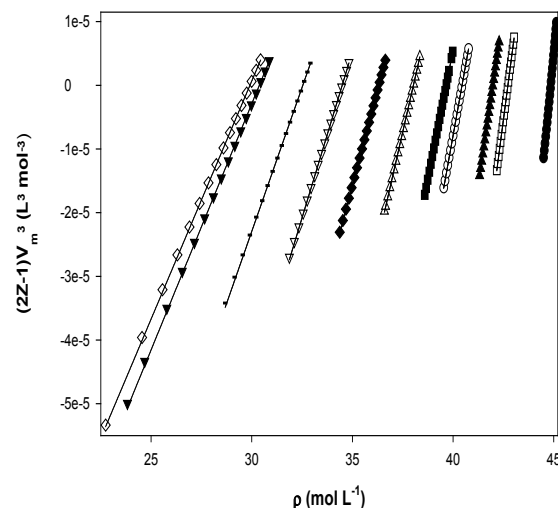


Fig.1. The GMA equation of state for fluorine [16]. The symbols are \bullet 56, \square 70, \blacktriangle 75, \circ 85, \blacksquare 90, \square 100, \square 110, \square 120, \square 130, \square 140, and \square 142 K.

It is interesting to analyze the capability of GMA equation of state to predict density and the volumetric behavior at liquid state for fluorine. There is a good (within experimental error) correspondence between these calculations and measured densities [16]. To calculate the density of liquid fluorine, the coefficients reported above can be used in the

following relation:

$$(B_0RT - 2B_1 + 2B_2T \ln T) \frac{\rho^5}{2} + (A_0RT - 2A_1 + 2A_2T \ln T) \frac{\rho^4}{2} + \frac{\rho RT}{2} - P = 0 \quad (4)$$

Remarkable is the pretty agreement in calculated density with the measurements, the absolute average percent deviation (

$$AAD = \frac{1}{N} \sum_{i=1}^N 100 \left| \frac{x_{cal} - x_{exp}}{x_{exp}} \right|$$

) for density is equal to 0.28%.

3.2. Thermodynamic Properties in Liquid State

3.2.1 Isobaric Expansion Coefficient

It is highly important to have knowledge of isothermal compressibility and isobaric expansion coefficient properties of fluorine as a function of temperature and pressure.

Isobaric expansion coefficient is:

$$\alpha = \frac{1}{V} \left(\frac{\partial V}{\partial T} \right)_P = - \frac{1}{\rho} \left(\frac{\partial \rho}{\partial T} \right)_P \quad (6)$$

where each symbol has the usual meaning. By differentiating GMA equation of state, we have derived a formula for calculating the thermal expansion and applied it to fluorine. Thus:

$$\alpha = \frac{(2B_1 + 2B_2T)\rho^5 + (2A_1 + 2A_2T)\rho^4 + 2P}{\rho RT^2 + 4\rho^4(A_0RT^2 - 2A_1T + 2A_2T^2 \ln T) + 5\rho^5(B_0RT^2 - 2B_1T + 2B_2T^2 \ln T)} \quad (7)$$

The isobaric expansion coefficient for F₂ from 56 K to 120 K under different pressures was calculated and Table 1 represents the results.

3.2.2 Isothermal Compressibility

The isothermal compressibility of a fluid can be calculated using the determined density data. We have calculated isothermal compressibility of fluorine at different conditions applying GMA equation of state and using the well-known equation:

$$\kappa = - \frac{1}{V} \left(\frac{\partial V}{\partial P} \right)_T = \frac{1}{\rho} \left(\frac{\partial \rho}{\partial P} \right)_T \quad (8)$$

Upon the calculation of isothermal compressibility, GMA equation of state correlated the density as a function of pressure, and isothermal compressibility was computed by differentiation. The derived relation is:

$$\kappa = \frac{2}{\rho RT + 4\rho^4(A_0RT - 2A_1 + 2A_2T \ln T) + 5\rho^5(B_0RT - 2B_1 + 2B_2T \ln T)} \quad (9)$$

The values of isothermal compressibility on different temperatures and pressures are displayed in Table 1 including the experimental densities.

3.2.3 Entropy

The residual entropy, S^{res} , is the entropy relative to the entropy of the ideal gas at the same temperature and pressure and defined as:

$$S^{res} = \int_0^{\rho} \frac{1}{\rho^2} \left[\left(\frac{\partial P}{\partial T} \right)_\rho - \rho R \right] d\rho \quad (10)$$

For the GMA equation of state, this yields:

$$S^{res} = \frac{R}{2} \ln \rho - (A_0R + 2A_1 \ln T + 2A_2) \frac{\rho^3}{6} - (B_0R + 2B_1 \ln T + 2B_2) \frac{\rho^4}{8} \quad (11)$$

The entropy can be calculated by adding the residual entropy to the entropy of the ideal diatomic gas [17] at the same temperature and pressure via the Sackur-Tetrede equation:

$$\frac{S}{R} = \frac{S^{res}}{R} + \ln \left[\left(\frac{2\pi MRT}{h^2 N^2} \right)^{3/2} \frac{e^{5/2}}{N\rho} \right] + \ln \left(\frac{8\pi^2 IRT}{2N h^2} \right) + \frac{h\nu}{kT} - \frac{1}{\exp\left(\frac{h\nu}{kT}\right) - 1} \quad (12)$$

$$\ln \left(1 - \exp\left(\frac{h\nu}{kT}\right) \right) + \ln w_{el}$$

Fig. 2 represents a comparison between the calculated entropies for F₂ and the experimental values as a function of temperature. As clearly shown in this figure, the calculated values are comparable with the experimental data (AAD = 9.42%).

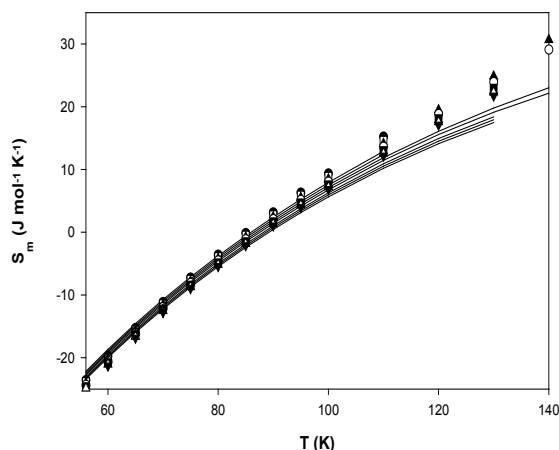


Fig. 2. The entropy, S_m , as a function of temperature. The symbols are \bullet 1, \square 4, \blacktriangle 7, \circ 10, \blacksquare 14, \triangle 17, \blacktriangledown 20 MPa. Solid line-equation of state, points-experiment [16].

3.2.4 Speed of Sound

The heat capacity ratio of a matter determines the speed of sound. The relation used to calculate speed of sound is:

$$w = \left[\gamma \left(\frac{\partial P}{\partial \rho} \right)_T \right]^{1/2} \quad (13)$$

where w is the speed of sound and γ is the ratio of heat capacities. Using GMA equation of state speed of sound is:

$$w = \left\{ \gamma \left[5\rho^4 \left(\frac{B_0 RT}{2} - B_1 + B_2 T \ln T \right) + 4\rho^3 \left(\frac{A_0 RT}{2} - A_1 + A_2 T \ln T \right) + \frac{RT}{2} \right] \right\}^{1/2} \quad (14)$$

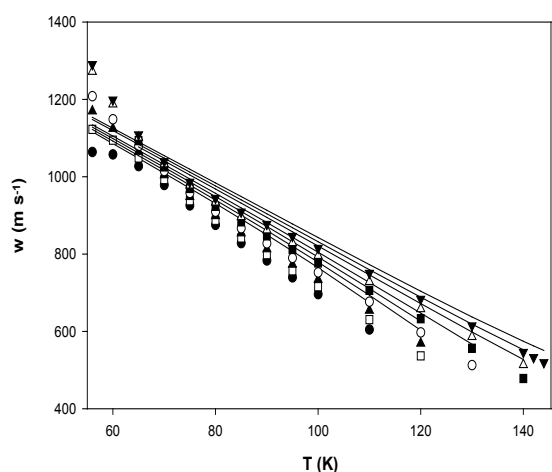


Fig. 3. Same as Figure 2 for speed of sound, w .

Fig. 3 shows the comparison of the calculated speed of sound and experimental

ones of fluorine against temperature (AAD = 5.05%).

3.2.5 Joule-Thomson Coefficient

The values of Joule-Thomson coefficient can be obtained from equations of state. Nonzero values of Joule-Thomson coefficient (μ_{JT}) directly reflect intermolecular interactions. To do so, we have:

$$\mu_{JT} = -\frac{1}{C_{P,m}} \left[V_m - T \left(\frac{\partial V_m}{\partial T} \right)_P \right] = \frac{T\alpha - 1}{\rho C_{P,m}} \quad (15)$$

where all symbols are known.

Fig. 4 is the comparison of the estimated and experimental Joule-Thomson coefficients for tested material against temperature (AAD = 4.84%).

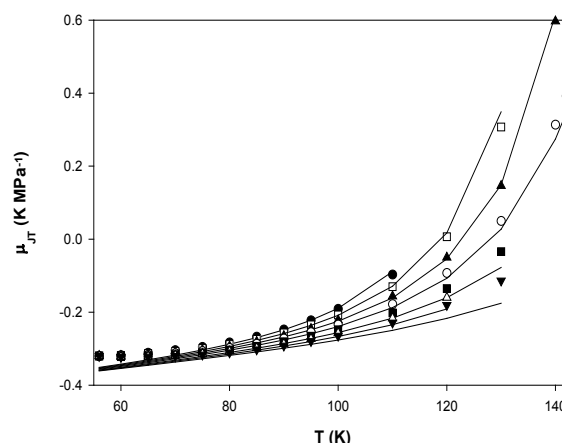


Fig. 4. Same as Figure 2 for Joule Thomson coefficient, μ_{JT}

3.2.6 Vapor-Liquid Equilibrium (Phase Diagram)

Under certain pressure and temperature conditions, a system can contain two or more phases in equilibrium. It can be summarized the solid-liquid-gas behavior of a substance by means of a phase diagram, which indicates under what conditions the various states of matter exist in equilibrium. To confirm the reliability of GMA equation of state, the VLE data for fluorine have been calculated and plotted at Fig. 5.

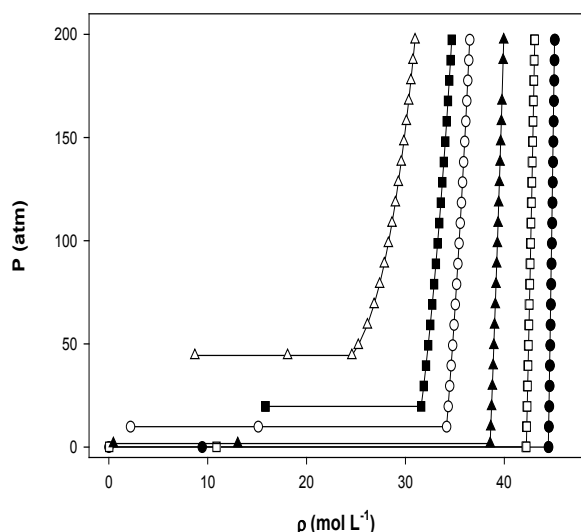


Fig. 5. Phase diagram, VLE, for fluorine. The symbols are ● 56, □ 70, ▲ 90, ○ 110, ■ 120, and △ 140 K.

4. Conclusions

In the present paper, the equation of state derived by Goharshadi *et al.* [11, 12] has been used to find selected thermophysical properties of liquid fluorine, and the results were compared with experimental values. We have compared our results with available experimental data for the pure fluorine [16].

Major attention was given to the extent GMA equation of state for fluorine and using this equation of state for calculation of physical and thermodynamic quantities such as density, isobaric expansion coefficient, isothermal compressibility, entropy, speed of sound, Joule-Thomson coefficient, and vapor-liquid equilibrium (VLE prediction) at 56-120 K and the pressure range at 0.05-20 MPa.

GMA equation of state covers the complete range of liquid state in the range up to 20 MPa and 120 K. It is admirable to note that the results are consistent with their reported counterparts. In addition, it is noticeable the acceptable agreement between our data and literature ones for properties of fluorine.

Acknowledgments

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Table 1. Isothermal compressibility and isobaric expansion coefficient for F₂

T(K)	P (MPa)	$\rho_{\text{exp}} \times 10^3$ (mol m ⁻³)	$\rho_{\text{cal}} \times 10^3$ (mol m ⁻³)	$\alpha \times 10^3$ (K ⁻¹)	$\kappa \times 10^5$ (atm ⁻¹)	T(K)	P (MPa)	$\rho_{\text{exp}} \times 10^3$ (mol m ⁻³)	$\rho_{\text{cal}} \times 10^3$ (mol m ⁻³)	$\alpha \times 10^3$ (K ⁻¹)	$\kappa \times 10^5$ (atm ⁻¹)
56	0.00051	44.49	44.46	3.38	7.65	65	0.00461	43.01	43.05	3.75	9.70
	1	44.53	44.49	3.35	7.59		0.5	43.03	43.07	3.73	9.65
	2	44.56	44.52	3.32	7.54		1	43.05	43.09	3.71	9.61
	3	44.60	44.56	3.29	7.49		2	43.09	43.14	3.67	9.53
	4	44.64	44.59	3.26	7.44		3	43.13	43.18	3.63	9.45
	5	44.67	44.62	3.23	7.39		4	43.17	43.22	3.59	9.37
	6	44.70	44.65	3.20	7.35		5	43.21	43.26	3.55	9.29
	7	44.74	44.69	3.17	7.30		6	43.25	43.30	3.51	9.22
	8	44.77	44.72	3.14	7.25		7	43.29	43.33	3.48	9.14
	9	44.80	44.75	3.11	7.21		8	43.33	43.37	3.44	9.07
	10	44.83	44.78	3.08	7.16		9	43.37	43.41	3.40	9.00
	11	44.86	44.81	3.05	7.11		10	43.41	43.45	3.37	8.92
	12	44.90	44.84	3.02	7.07		11	43.44	43.49	3.34	8.86
	13	44.93	44.88	2.99	7.03		12	43.48	43.53	3.30	8.79
	14	44.96	44.91	2.97	6.98		13	43.52	43.56	3.27	8.72
	15	44.98	44.94	2.94	6.94		14	43.55	43.60	3.24	8.65
	16	45.01	44.97	2.91	6.90		15	43.59	43.64	3.20	8.59
	17	45.04	45.00	2.89	6.86		16	43.63	43.68	3.17	8.52
	18	45.07	45.03	2.86	6.82		17	43.66	43.71	3.14	8.46
	19	45.10	45.06	2.83	6.78		18	43.70	43.75	3.11	8.40
	20	45.13	45.09	2.81	6.74		19	43.73	43.78	3.08	8.34
60	0.00149	43.83	43.84	3.54	8.48		20	43.77	43.82	3.05	8.28
	0.1	43.83	43.85	3.53	8.47	70	0.01198	42.17	42.23	3.98	11.15
	1	43.87	43.88	3.50	8.42		1	42.22	42.28	3.93	11.04
	2	43.91	43.92	3.47	8.35		2	42.26	42.32	3.88	10.93
	3	43.94	43.95	3.43	8.29		3	42.31	42.37	3.84	10.83
	4	43.98	43.99	3.40	8.23		4	42.36	42.41	3.80	10.72
	5	44.02	44.03	3.36	8.17		5	42.40	42.46	3.75	10.62
	6	44.05	44.06	3.33	8.11		6	42.45	42.50	3.71	10.52
	7	44.09	44.10	3.30	8.05		7	42.49	42.55	3.67	10.42
	8	44.12	44.13	3.27	8.00		8	42.53	42.59	3.63	10.33
	9	44.16	44.17	3.24	7.94		9	42.58	42.63	3.59	10.23
	10	44.19	44.20	3.20	7.88		10	42.62	42.68	3.55	10.14
	11	44.23	44.23	3.17	7.83		11	42.66	42.72	3.51	10.05
	12	44.26	44.27	3.14	7.78		12	42.70	42.76	3.47	9.96
	13	44.29	44.30	3.11	7.72		13	42.75	42.80	3.43	9.88
	14	44.32	44.34	3.08	7.67		14	42.79	42.84	3.40	9.79
	15	44.36	44.37	3.05	7.62		15	42.83	42.89	3.36	9.71
	16	44.39	44.40	3.02	7.57		16	42.87	42.93	3.32	9.63
	17	44.42	44.44	3.00	7.52		17	42.91	42.97	3.29	9.55
	18	44.45	44.47	2.97	7.47		18	42.95	43.01	3.26	9.47
	19	44.48	44.50	2.94	7.42		19	42.99	43.05	3.22	9.39
	20	44.51	44.53	2.91	7.38		20	43.03	43.09	3.19	9.32

Table 1. Continued

T(K)	P (MPa)	$\rho_{\text{exp}} \times 10^3$ (mol m ⁻³)	$\rho_{\text{cal}} \times 10^3$ (mol m ⁻³)	$\alpha \times 10^3$ (K ⁻¹)	$\kappa \times 10^5$ (atm ⁻¹)	T(K)	P (MPa)	$\rho_{\text{exp}} \times 10^3$ (mol m ⁻³)	$\rho_{\text{cal}} \times 10^3$ (mol m ⁻³)	$\alpha \times 10^3$ (K ⁻¹)	$\kappa \times 10^5$ (atm ⁻¹)
75	0.02706	41.32	41.37	4.23	12.91	85	0.1009	39.53	39.55	4.84	17.74
1		41.37	41.43	4.18	12.77	1		39.60	39.61	4.77	17.48
2		41.42	41.48	4.13	12.62	2		39.67	39.68	4.69	17.21
3		41.47	41.53	4.07	12.48	3		39.73	39.75	4.62	16.94
4		41.53	41.58	4.02	12.34	4		39.80	39.81	4.55	16.69
5		41.58	41.63	3.97	12.21	5		39.87	39.88	4.48	16.44
6		41.63	41.68	3.92	12.07	6		39.93	39.94	4.41	16.20
7		41.68	41.73	3.88	11.95	7		40.00	40.00	4.35	15.97
8		41.73	41.78	3.83	11.82	8		40.06	40.07	4.28	15.75
9		41.78	41.83	3.78	11.70	9		40.13	40.13	4.22	15.53
10		41.83	41.88	3.74	11.58	10		40.19	40.19	4.16	15.32
11		41.87	41.92	3.69	11.46	11		40.25	40.25	4.10	15.12
12		41.92	41.97	3.65	11.35	12		40.31	40.31	4.04	14.92
13		41.97	42.02	3.61	11.23	13		40.37	40.37	3.99	14.72
14		42.02	42.06	3.57	11.13	14		40.43	40.43	3.93	14.54
15		42.06	42.11	3.53	11.02	15		40.49	40.49	3.88	14.36
16		42.11	42.16	3.49	10.91	16		40.54	40.54	3.83	14.18
17		42.15	42.20	3.45	10.81	17		40.60	40.60	3.78	14.01
18		42.20	42.25	3.41	10.71	18		40.66	40.65	3.73	13.84
19		42.24	42.29	3.37	10.61	19		40.71	40.71	3.68	13.68
20		42.29	42.33	3.33	10.52	20		40.77	40.76	3.64	13.52
80	0.05467	40.44	40.48	4.52	15.07	90	0.17296	38.59	38.57	5.21	21.10
1		40.50	40.54	4.46	14.87	1		38.66	38.64	5.13	20.77
2		40.56	40.60	4.39	14.68	2		38.74	38.72	5.04	20.38
3		40.62	40.66	4.33	14.48	3		38.82	38.79	4.95	20.01
4		40.68	40.71	4.27	14.30	4		38.89	38.87	4.86	19.65
5		40.74	40.77	4.21	14.12	5		38.97	38.95	4.77	19.31
6		40.79	40.83	4.16	13.94	6		39.05	39.02	4.69	18.98
7		40.85	40.88	4.10	13.77	7		39.12	39.09	4.62	18.66
8		40.91	40.94	4.05	13.60	8		39.19	39.16	4.54	18.35
9		40.96	40.99	3.99	13.44	9		39.26	39.23	4.47	18.06
10		41.02	41.05	3.94	13.28	10		39.33	39.30	4.40	17.78
11		41.07	41.10	3.89	13.13	11		39.40	39.37	4.33	17.50
12		41.13	41.15	3.84	12.98	12		39.47	39.44	4.26	17.24
13		41.18	41.21	3.79	12.83	13		39.54	39.51	4.20	16.98
14		41.23	41.26	3.75	12.69	14		39.60	39.57	4.13	16.73
15		41.28	41.31	3.70	12.55	15		39.67	39.64	4.07	16.49
16		41.33	41.36	3.65	12.42	16		39.73	39.70	4.01	16.26
17		41.39	41.41	3.61	12.28	17		39.80	39.76	3.96	16.03
18		41.44	41.46	3.57	12.15	19		39.92	39.89	3.84	15.60
19		41.49	41.51	3.52	12.03	20		39.98	39.95	3.79	15.40
20		41.53	41.56	3.48	11.90	95	0.27894	37.61	37.55	5.63	25.41

Table 1. Continued

T(K)	P (MPa)	$\rho_{\text{exp}} \times 10^3$ (mol m ⁻³)	$\rho_{\text{cal}} \times 10^3$ (mol m ⁻³)	$\alpha \times 10^3$ (K ⁻¹)	$\kappa \times 10^5$ (atm ⁻¹)	T(K)	P (MPa)	$\rho_{\text{exp}} \times 10^3$ (mol m ⁻³)	$\rho_{\text{cal}} \times 10^3$ (mol m ⁻³)	$\alpha \times 10^3$ (K ⁻¹)	$\kappa \times 10^5$ (atm ⁻¹)
1		37.68	37.62	5.55	24.98						
2		37.77	37.71	5.43	24.42	110	1	34.37	34.16	7.45	48.80
3		37.86	37.80	5.32	23.88		2	34.53	34.33	7.16	46.61
4		37.95	37.89	5.21	23.37		3	34.68	34.48	6.91	44.63
5		38.04	37.97	5.11	22.89		4	34.82	34.63	6.67	42.84
6		38.12	38.06	5.01	22.42		5	34.96	34.77	6.45	41.20
7		38.21	38.14	4.91	21.98		6	35.10	34.91	6.25	39.69
8		38.29	38.23	4.82	21.56		7	35.23	35.05	6.06	38.31
9		38.37	38.31	4.74	21.15		8	35.36	35.18	5.89	37.02
10		38.45	38.39	4.65	20.76		9	35.48	35.30	5.72	35.83
11		38.53	38.46	4.57	20.39		10	35.60	35.43	5.57	34.73
12		38.61	38.54	4.49	20.03		11	35.71	35.55	5.42	33.69
13		38.68	38.62	4.42	19.68		12	35.83	35.66	5.29	32.73
14		38.75	38.69	4.34	19.35		13	35.94	35.78	5.16	31.82
15		38.83	38.76	4.27	19.03		14	36.04	35.89	5.04	30.97
16		38.90	38.84	4.20	18.72		15	36.15	36.00	4.92	30.16
17		38.97	38.91	4.14	18.43		16	36.25	36.10	4.81	29.40
18		39.04	38.98	4.07	18.14		17	36.35	36.21	4.71	28.69
19		39.11	39.05	4.01	17.86		18	36.45	36.31	4.61	28.01
20		39.17	39.11	3.95	17.59		19	36.54	36.41	4.51	27.36
							20	36.63	36.50	4.42	26.75
100	0.5	36.59	36.48	6.12	30.98						
	1	36.65	36.54	6.05	30.53	120	2	31.87	31.60	9.45	84.17
	2	36.75	36.65	5.89	29.69		3	32.11	31.85	8.86	77.65
	3	36.86	36.75	5.75	28.89		4	32.34	32.09	8.35	72.17
	4	36.96	36.86	5.62	28.15		5	32.55	32.31	7.92	67.51
	5	37.07	36.96	5.49	27.44		6	32.75	32.52	7.53	63.47
	6	37.16	37.06	5.36	26.77		7	32.95	32.72	7.19	59.94
	7	37.26	37.16	5.25	26.14		8	33.13	32.91	6.89	56.83
	8	37.35	37.25	5.14	25.54		9	33.30	33.09	6.61	54.05
	9	37.45	37.34	5.03	24.97		10	33.47	33.26	6.36	51.56
	10	37.54	37.43	4.93	24.43		11	33.62	33.43	6.14	49.32
	11	37.63	37.52	4.83	23.92		12	33.78	33.58	5.93	47.28
	12	37.71	37.61	4.74	23.42		13	33.92	33.74	5.74	45.42
	13	37.80	37.70	4.65	22.95		14	34.07	33.89	5.56	43.71
	14	37.88	37.78	4.56	22.50		15	34.20	34.03	5.39	42.14
	15	37.96	37.87	4.48	22.07		16	34.34	34.17	5.24	40.69
	16	38.04	37.95	4.40	21.66		17	34.47	34.31	5.09	39.35
	17	38.12	38.03	4.32	21.27		18	34.59	34.44	4.96	38.10
	18	38.20	38.11	4.25	20.89		19	34.71	34.56	4.83	36.93
	19	38.27	38.18	4.18	20.52		20	34.83	34.69	4.71	35.84
	20	38.35	38.26	4.11	20.17						

List of Symbols

e	Neper's number
h	Plank's constant
I	moment inertia
k	Boltzmann's constant
M	molar weight
N	Avogadro's number
P	pressure
R	universal gas constant
S	entropy
T	absolute temperature
V	volume
w	speed of sound
w_{el}	the ground electronic state degeneracy
Z	compression factor

Greek Letters

α	isobaric expansion coefficient
γ	ratio of isobaric and isochoric heat capacities
κ	isothermal compressibility
μ_{JT}	Joule-Thomson coefficient
ν	vibration frequency
ρ	molar density

Subscripts

c	critical
cal	calculated
exp	experimental
m	molar

Superscripts

Res	residual
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