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THERMODYNAMIC PROPERTIES OF GASEOUS ETHANE AND ETHENE+

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Based on the most probable values and additional recommended values proposed by the High Pressure Data Center of Japan, new equations of state for gaseous ethane and ethene are devised for the range of temperatures 273.15 K to 498.15 K and of pressures up to 30 MPa for ethane and for the range of temperatures 273.15 K to 423.15 K and of pressures up to 80 MPa for ethene. The canonical functions are also derived from the new equations of state, and the thermodynamic property values are calculated by differentiating these functions. The calculated values of compressibility factor, molar volume, molar enthalpy and molar entropy are tabulated in this paper.

Introduction

According to the critical evaluation of the P-V-T data, the most probable values of compressibility factor for gaseous ethane and ethene were proposed by the High Pressure Data Center of Japan (HPDCJ) organized in the Society of Material Science, Japan, under the sponsorship of the Agency of Science and Technology[1]. As the next program of the HPDCJ, new equations of state for both ethane and ethene are formulated based on these most probable values in order to calculate the P-V-T property values as well as other thermodynamic property values at respective states. In the present paper, new equations of state which cover the range of temperatures 273.15 K to 498.15 K and of pressures up to 30 MPa for ethane and that of temperatures 273.15 K to 423.15 K and of pressures up to 80 M Pa for ethene are described and the tables of thermodynamic property values are presented.

New equations of state

The skeleton table values of compressibility factor for gaseous ethane and ethene which were proposed by the HPDCJ cover the ranges shown in Figs. 1 and 2, respectively. These skeleton table values accompanied with estimated uncertainties are classified into two groups, such as the most pro-

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1) K. Date, K. Watanabe, and M. Uematsu, *This Journal*, 43, 92 (1973)

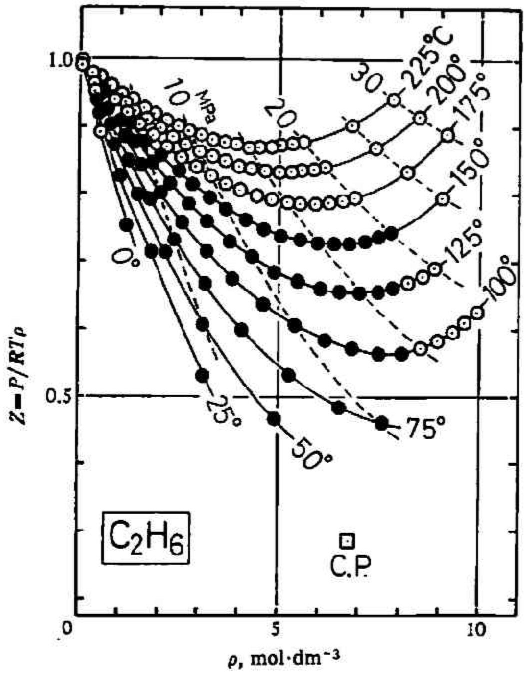

Fig. 1 The most probable values and additional recommended values for ethane
●: most probable value
⊙: additional recommended value
□: critical point (305.43 K, 4.880 MPa, 6.75 mol·dm^{-3})[2)]

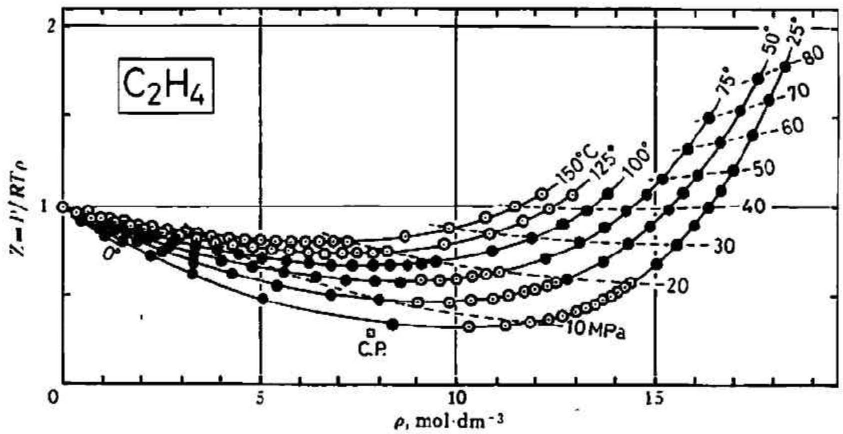

Fig. 2 The most probable values and additional recommended values for ethene
●: most probable value, ⊙: additional recommended value
□: critical point (282.36 K, 5.032 MPa, 7.77 mol·dm^{-3})[2)]

bable values and additional recommended values, according to the derivation of these values. Both the most probable and additional recommended values were used as the basic data in the present study of devising new equations of state.

Because of the wide ranges of parameters as shown in Figs. 1 and 2, density and temperature are chosen as independent variables. As is well known, Benedict-Webb-Rubin (BWR) equation of state, which expresses pressure as a function of density and temperature, describes well the P-V-T properties of hydrocarbons. However, the BWR equation is limited in its validity in a maximum reduced density of about 1.5 excluding the critical region owing to the fact that it has only 8 constants. Although the skeleton table for ethane covers the region of reduced density less than 1.5 and excluding the critical region, that for ethene is extended up to about 2.7 times larger than the critical density[2)]. Therefore, additional terms are required to describe accurately the P-V-T properties of ethene. After several possible additional terms had been applied, the following functional form, which was developed from the original BWR equation, was adopted for the present purpose:

$$\begin{aligned} P= & RT\rho+(a_1T+a_2+a_3/T^2)\rho^2 \\ & +(a_4T+a_5)\rho^3 \\ & +(a_6+a_7/T^5)\rho^4 \\ & +(a_8+a_9/T^3)\rho^5 \\ & +(a_{10}+a_{11}/T)\rho^6 \\ & +(a_{12}+a_{13}/T^2+a_{14}/T^4)(1+\gamma\rho^2)\rho^3\exp(-\gamma\rho^2). \end{aligned} \quad (1)$$

where P=pressure in MPa,

R=molar gas constant in $\mathrm{J \cdot K^{-1} mol^{-1}}$,

T=temperature in K, $T=t+273.15$,

t=temperature in °C on IPTS-68,

ρ=molar density in $\mathrm{mol \cdot cm^{-3}}$,

$a_1, a_2, \cdots, a_{14}, \gamma$=numerical constants.

Table 1 Numerical constants in Eqs. (1) and (2) for ethane and ethene

	Ethane	Ethene
γ	1.2658363×10^{4}	1.3929979×10^{4}
a_1	5.0639348×10^{2}	5.7505391×10^{2}
a_2	-4.0180384×10^{5}	-3.9857311×10^{5}
a_3	-1.8913502×10^{10}	-1.0630701×10^{10}
a_4	8.4222162×10^{4}	4.0629605×10^{4}
a_5	-3.1167109×10^{7}	-3.0058264×10^{6}
a_6	0	2.3489094×10^{8}
a_7	0	6.8649318×10^{20}
a_8	0	-2.8650224×10^{10}
a_9	0	-6.3746747×10^{17}
a_{10}	9.0228835×10^{12}	4.1892581×10^{12}
a_{11}	0	-1.0768430×10^{14}
a_{12}	0	-7.7042510×10^{6}
a_{13}	3.0699808×10^{12}	1.5572266×10^{12}
a_{14}	0	-1.3328900×10^{16}
A_1	1.7464272×10^{3}	1.6711271×10^{2}
A_2	-1.7468344×10^{0}	5.2608796×10^{0}
A_3	1.7907139×10^{-1}	1.4293953×10^{-1}
A_4	-5.3644526×10^{-5}	-5.4900378×10^{-5}

2) A.P. Kudchadker, G. H. Alani, and B. J., Zwolinski, *Chem. Rev.*, **68**, 659 (1968)

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Table 2 Average deviations from Eq. (1)

	Author	Number of data points	Average deviation (%)*
Ethane	Skeleton table values[1]	157	0.082
	Douslin and Harrison (73)[6]	132	0.143**
	Michels *et al.* (54)[7]	89	0.085
	Reamer *et al.* (44)[8]	65	0.259
	Beattie *et al.* (39)[9]	54	0.140
	Sage *et al.* (37)[10]	148	0.406
	Beattie *et al.* (35)[11]	82	0.322
Ethene	Skeleton table values[1]	170	0.060
	Lee and Edmister (70)[12]	70	0.772
	Sass *et al.* (67)[13]	29	0.194
	Ku and Dodge (67)[14]	25	0.242
	Thomas and Zander (66)[15]	30	0.052
	Walters *et al.* (54)[16]	139	0.167
	Michels *et al.* (42)[17]	217	0.091
	Michels *at al.* (36)[18]	103	0.088

* Calculated by

$$\sigma\,[\%] = \frac{\sum |(Z_{\mathrm{exp}} - Z_{\mathrm{cal}})/Z_{\mathrm{cal}}| \times 100}{n},$$

where Z_{exp} = original experimental values of compressibility factor,
Z_{cal} = calculated values by Eq. (1),
n = number of data points.

** Skeleton table values had been already determined, before these data were published.

The following values were adopted as the atomic weights recommended by IUPAC[3] and molar gas constant recommended by CODATA[4]:

$C = 12.011 \pm 0.001$,

$H = 1.0079 \pm 0.0001$,

$R = 8.31441 \pm 0.00026$ ($J\cdot K^{-1}\cdot mol^{-1}$).

In order to determine the numerical constants in Eq. (1), the skeleton table values were introduced as a set of input data into a least-squares procedure and the characteristics of the computed C_p values were also examined. In consequence of this procedure, the numerical constants for both ethane and ethene in Eq. (1) were fixed on as listed in Table 1.

When the C_p values were computed, the following $C_p{}^0$ correlations for ethane and ethene which were newly correlated based on the values recommended by Touloukian and Makita[5] were used:

$$C_p{}^0 = A_1/T + A_2 + A_3T + A_4T^2. \tag{2}$$

3) *Pure and Appl. Chem.*, **37**, 589 (1974)

4) *CODATA Bull.*, No.11 (1973)

5) Y. S. Touloukian, and T. Makitan, "Specific Heat-Nonmetallic Liquids and Gases, (Thermophysical Properties of Matters)", The TPRC Data Series vol. 6, IFI/PLENUM, New York (1970)

This C_p^0 correlations in $J \cdot K^{-1} mol^{-1}$ reproduce the C_p^0 values recommended by Touloukian and Makita within the deviation of 0.03% for the range of temperatures 273.15 K to 573.15 K both for ethane and ethene. The numerical constants in Eq. (2) are also tabulated in Table 1.

Comparison of the compressibility factor values computed from Eq. (1) with the skeleton table values and experimental data of both ethane[6~11] and ethene[12~18] was shown in detail in the previous paper[19]. Table 2 shows that the computed values are in satisfactory agreement with the skeleton table values and experimental data[7,17,18] which were evaluated to be the most reliable by the HPDCJ[1]. The computed compressibility factor values as well as their comparison with the skeleton table values are tabulated for ethane and ethene in Tables 3 and 4, respectively.

As for experimental C_p data of ethane and ethene, there do not exist any reliable C_p data except that of Bier *et al.*[20]. for ethane as far as our present survey could determine. The average percentage deviation of these C_p data from the computed C_p values is 0.73% (61 data points) by using the same C_p^0 values.

Canonical function

When density and temperature are chosen as the independent variables. the expressions for pressure and all other thermodynamic properties can be derived directly by the partial differentiation of the canonical function $A=A(\rho, T)$, where A is molar Helmholtz function. In the present study, molar Helmholtz function A in $J \cdot mol^{-1}$ is derived from Eqs. (1) and (2) as follows:

$$\begin{aligned} A = & B_0 + B_1 T + B_2 T^2 + B_3 T^3 + B_4 \ln T + B_5 T \ln T \\ & + RT \ln \rho \\ & + (b_1 T + b_2 + b_3 / T^2)\rho \\ & + (b_4 T + b_5)\rho^2 \\ & + (b_6 + b_7 / T^5)\rho^3 \\ & + (b_8 + b_9 / T^3)\rho^4 \end{aligned}$$

6) D. R. Douslin, and R. H. Harrison, *J. Chem. Thermodynamics*, **5**, 491 (1973)
7) A. Michels, W. Van Straaten, and J. Dawson, *Physica*, **20**, 17 (1954)
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19) M. Uematsu, S. Saegusa, K. Watanabe, and I. Tanishita, Proceedings of the 4th International Conference on High Pressure, Kyoto, Japan, November, 1974, p.561
20) K. Bier, G. Maurer *et al.*, Private communication, will be published in *Chemical Engineering Science*, vol. 30 (1975)

Table 5 Numerical constants in Eq. (3) for ethane and ethene

	Ethane	Ethene
B_0	-1.5168402×10^{4}	-8.2217326×10^{3}
B_1	6.1635642×10^{1}	1.0307823×10^{2}
B_2	-8.9535695×10^{-2}	-7.1469765×10^{-2}
B_3	8.9407543×10^{-5}	9.1500630×10^{-6}
B_4	1.7464272×10^{3}	1.6711271×10^{2}
B_5	1.0061244×10^{1}	3.0535304×10^{0}
γ	1.2658363×10^{4}	1.3929979×10^{4}
b_1	5.0639348×10^{2}	5.7505391×10^{2}
b_2	-4.0180384×10^{5}	-3.9857311×10^{5}
b_3	-1.8913502×10^{10}	-1.0630701×10^{10}
b_4	4.2111081×10^{4}	2.0314802×10^{4}
b_5	-1.5583555×10^{7}	-1.5029132×10^{6}
b_6	0	7.8296980×10^{7}
b_7	0	2.2883106×10^{20}
b_8	0	-7.1625560×10^{9}
b_9	0	-1.5936687×10^{17}
b_{10}	1.8045767×10^{12}	8.3785162×10^{11}
b_{11}	0	-2.1536860×10^{13}
b_{12}	0	-7.7042510×10^{6}
b_{13}	3.0699808×10^{12}	1.5572266×10^{12}
b_{14}	0	-1.3328900×10^{16}

$$+(b_{10}+b_{11}/T)\rho^5$$
$$+(b_{12}+b_{13}/T^2+b_{14}/T^4)[1/\gamma-(\rho^2/2+1/\gamma)\exp(-\gamma\rho^2)]. \quad (3)$$

The numerical constants in Eq. (3) are listed in Table 5. The numerical values of B_0 and B_1 in Eq. (3) are fixed due to the following conditions:

(i) $S=0$ (J·K^{-1}mol^{-1}) at 298.15 K and 0.101325 MPa,

(ii) $H=0$ (J·mol^{-1}) at 298.15 K and 0 MPa.

Derived functions

According to the general thermodynamic relations, the pressuse P in MPa, the molar entropy S in J·K^{-1} mol^{-1}, the molar enthalpy H in J·mol^{-1}, the molar heat capacity at constant volume C_v in J·K^{-1} mol^{-1} and the molar heat capacity at constant pressure C_p in J·K^{-1}mol^{-1} can be calculated by the following expressions:

$$P=\rho^2(\partial A/\partial\rho)_T, \quad (4)$$

$$S=-(\partial A/\partial T)_\rho, \quad (5)$$

$$H=A-T(\partial A/\partial T)_\rho+\rho(\partial A/\partial\rho)_T, \quad (6)$$

$$C_v=-T(\partial^2 A/\partial T^2)_\rho, \quad (7)$$

$$C_p=T[-(\partial^2A/\partial T^2)_\rho+\frac{\rho(\partial^2A/\partial\rho\partial T)^2}{2(\partial A/\partial\rho)_T+\rho(\partial^2A/\partial\rho^2)_T}]. \quad (8)$$

In addition, the compressibility factor Z and the molar volume V in $cm^3\ mol^{-1}$ can be calculated from Eqs. (9) and (10), respectively.

$$Z=P/RT\rho \quad (9)$$

$$V=1/\rho \quad (10)$$

Calculated thermodynamic properties

By differentiating the new equations of state expressed in the canonical forms for gaseous ethane and ethene, Eq. (3), thermodynamic properties are calculated. The calculated molar volume, the molar enthalpy and the molar entropy both for ethane and ethene are tabulated in Tables 6 and 7, respectively.

Conclusion

As a part of the activity of the High Pressure Data Center of Japan, new equations of state, Eq. (1), both for gaseous ethane and ethene are formulated based on the most probable values and additional recommended values proposed by the HPDCJ. These values cover the range of temperatures 273.15 K to 498.15 K and of pressures up to 30 MPa for ethane and that of temperatures 273.15 K to 423.15 K and of pressures up to 80 MPa for ethene. The thermodynamic property values in these ranges can be calculated by differentiating the canonical functions, Eq. (3), for both ethane and ethene which are derived from the new equations of state. The calculated values of the compressibility factor, the molar volume, the molar enthalpy and the molar entropy are tabulated in Tables 3, 4, 6 and 7.

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Table 3 Calculated values of the compressibility factor, Z, for gaseous ethane and their comparison with the skeleton table values

Pressure MPa (atm)		Temperature K (°C) 273.15 (0)	298.15 (25)	323.15 (50)	348.15 (75)	373.15 (100)	398.15 (125)	423.15 (150)	448.15 (175)	473.15 (200)	498.15 (225)
0.101325	(1)	0.99003 0.98977 0.026/0.030	0.99233 0.99232 0.001/0.030	0.99406 0.99409 -0.003/0.030	0.99534 0.99538 -0.003/0.030	0.99628 0.99632 -0.004/0.030	0.99699 0.99703 -0.005/0.030	0.99755 0.99760 -0.005/0.030	0.99799 0.99804 -0.005/0.030	0.99837 0.99839 -0.002/0.030	0.99870 0.99867 0.003/0.030
1.0133	(10)	0.8921 0.88947 0.294/0.10	0.9199 0.91911 0.086/0.12	0.9386 0.93884 -0.026/0.09	0.9523 0.95266 -0.038/0.17	0.9623 0.96270 -0.042/0.20	0.9697 0.97021 -0.052/0.15	0.9755 0.97595 -0.046/0.17	0.9800 0.98043 -0.043/0.20	0.9835 0.98398 -0.048/0.30	0.9864 0.98683 -0.044/0.30
2.0265	(20)	0.7522 0.74962 0.343/0.10	0.8268 0.82621 0.071/0.12	0.8718 0.87213 -0.037/0.10	0.9025 0.90265 -0.017/0.17	0.9237 0.92416 -0.050/0.20	0.9387 0.93993 -0.131/0.14	0.9502 0.95183 -0.171/0.16	0.9593 0.96102 -0.179/0.20	0.9662 0.96825 -0.212/0.30	0.9726 0.97403 -0.147/0.30
3.0398	(30)		0.7125 0.71204 0.064/0.12	0.7976 0.79775 -0.019/0.10	0.8491 0.84946 -0.042/0.17	0.8836 0.88432 -0.081/0.17	0.9084 0.90923 -0.091/0.12	0.9269 0.92773 -0.090/0.16	0.9400 0.94186 -0.198/0.25	0.9510 0.95290 -0.199/0.35	0.9603 0.96166 -0.141/0.40
4.0530	(40)		0.5301 0.53773 -1.439/0.12	0.7116 0.71194 -0.048/0.10	0.7921 0.79247 -0.047/0.16	0.8426 0.84315 -0.066/0.15	0.8776 0.87822 -0.071/0.12	0.9031 0.90378 -0.076/0.15	0.9212 0.92307 -0.203/0.30	0.9363 0.93800 -0.181/0.40	0.9486 0.94978 -0.124/0.45
5.0662	(50)			0.6069 0.60676 0.024/0.10	0.7312 0.73105 0.020/0.15	0.8006 0.80079 -0.024/0.15	0.8463 0.84710 -0.094/0.11	0.8793 0.88015 -0.096/0.15	0.9033 0.90476 -0.162/0.30	0.9235 0.92365 -0.016/0.40	0.9382 0.93846 -0.028/0.55
6.0795	(60)			0.4664 0.46346 0.630/0.11	0.6664 0.66495 0.217/0.14	0.7576 0.75759 0.001/0.14	0.8157 0.81617 -0.058/0.11	0.8566 0.85704 -0.051/0.15	0.8865 0.88709 -0.066/0.35	0.9097 0.90995 -0.027/0.40	0.9274 0.92778 -0.041/0.55
7.0928	(70)				0.5976 0.59590 0.285/0.13	0.7146 0.71441 0.026/0.13	0.7859 0.78590 -0.001/0.11	0.8347 0.83474 -0.005/0.15	0.8697 0.87022 -0.060/0.35	0.8969 0.89702 -0.013/0.40	0.9178 0.91780 -0.000/0.55
8.1060	(80)				0.5327 0.53146 0.232/0.12	0.6735 0.67288 0.092/0.12	0.7571 0.75697 0.018/0.11	0.8135 0.81359 -0.011/0.15	0.8541 0.85437 -0.031/0.35	0.8853 0.88497 0.037/0.40	0.9092 0.90861 0.065/0.55
9.1192	(90)				0.4849 0.48495 -0.011/0.11	0.6365 0.63552 0.154/0.12	0.7306 0.73022 0.052/0.11	0.7942 0.79399 0.027/0.15	0.8396 0.83973 -0.015/0.35	0.8744 0.87393 0.053/0.40	0.9003 0.90028 0.002/0.50

10.133	(100)	0.4618 0.46189 -0.020/0.10	0.6059 0.60519 0.118/0.13	0.7072 0.70663 0.081/0.11	0.7767 0.77635 0.045/0.15	0.8264 0.82651 -0.013/0.35	0.8643 0.86402 0.033/0.40	0.8933 0.89287 0.048/0.50
11.146	(110)		0.5839 0.58375 0.026/0.15	0.6873 0.68709 0.031/0.11	0.7614 0.76107 0.043/0.15	0.8151 0.81492 0.022/0.35	0.8557 0.85533 0.043/0.40	0.8866 0.88645 0.017/0.50
12.159	(120)		0.5713 0.57131 0.002/0.17	0.6720 0.67218 -0.027/0.11	0.7484 0.74848 -0.010/0.14	0.8056 0.80512 0.059/0.40	0.8485 0.84796 0.064/0.40	0.8812 0.88106 0.016/0.50
13.172	(130)		0.5668 0.56665 0.027/0.19	0.6612 0.66207 -0.132/0.11	0.7391 0.73876 0.046/0.14	0.7972 0.79724 -0.004/0.35	0.8423 0.84197 0.039/0.40	0.8766 0.87673 -0.015/0.45
14.186	(140)		0.5678 0.56813 -0.059/0.23	0.6555 0.65652 -0.155/0.12	0.7320 0.73198 0.003/0.14	0.7912 0.79312 -0.015/0.25	0.8377 0.83741 0.035/0.40	0.8732 0.87350 -0.034/0.45
15.199	(150)		0.5738 0.57426 -0.080/0.27	0.6540 0.65504 -0.158/0.13	0.7275 0.72805 -0.075/0.13	0.7886 0.78737 0.155/0.20	0.8342 0.83428 -0.009/0.40	0.8707 0.87135 -0.075/0.45
16.212	(160)		0.5835 0.58381 -0.053/0.32	0.6568 0.65705 -0.038/0.16	0.7259 0.72678 -0.120/0.13	0.7862 0.78535 0.108/0.20	0.8322 0.83256 -0.043/0.40	0.8694 0.87029 -0.103/0.45
17.225	(170)		0.5957 0.59588 -0.030/0.35	0.6618 0.66198 -0.027/0.18	0.7270 0.72792 -0.126/0.13	0.7859 0.78515 0.096/0.20	0.8335 0.83221 0.155/0.30	0.8689 0.87029 -0.160/0.40
18.239	(180)		0.6104 0.60980 0.099/0.39	0.6694 0.66931 0.013/0.20	0.7302 0.73121 -0.138/0.13	0.7869 0.78664 0.033/0.20	0.8348 0.83316 0.196/0.25	0.8729 0.87130 0.183/0.25
19.252	(190)		0.6250 0.62508 -0.013/0.44	0.6789 0.67861 0.043/0.20	0.7358 0.73638 -0.079/0.13	0.7900 0.78968 0.040/0.20	0.8366 0.83535 0.149/0.25	0.8744 0.87329 0.126/0.25
20.265	(200)			0.6900 0.68949 0.074/0.20	0.7426 0.74318 -0.078/0.13	0.7943 0.79414 0.020/0.20	0.8396 0.83869 0.109/0.25	0.8768 0.87621 0.067/0.25
25.331	(250)				0.7954 0.79460 0.101/0.20	0.8330 0.83280 0.024/0.20	0.8693 0.86951 -0.024/0.25	0.9021 0.90263 -0.058/0.25
30.398	(300)					0.8895 0.88926 0.028/0.20	0.9163 0.91704 -0.080/0.25	0.9425 0.94387 -0.145/0.25

[- - -] : the most probable values

1st line: skeleton table value, Z_{ST}

2nd line: calculated value, Z_{cal}

3rd line: deviation (%) / uncertainty (%)

(deviation = $[(Z_{ST} - Z_{cal}) / Z_{cal}] \times 100$)

Table 4 Calculated values of the compressibility factor, Z, for gaseous ethene and their comparison with the skeleton table values

Pressure MPa (atm)	Temperature K (°C) 273.15 (0)	298.15 (25)	323.15 (50)	348.15 (75)	373.15 (100)	398.15 (125)	423.15 (150)
0.101325 (1)	0.99242 0.99242 0.000/0.030	0.99443 0.99426 0.017/0.030	0.99571 0.99557 0.014/0.030	0.99661 0.99654 0.008/0.030	0.99727 0.99726 0.001/0.030	0.99779 0.99781 -0.002/0.030	0.99822 0.99824 -0.002/0.030
1.0133 (10)	0.9215 0.91999 0.163/0.10	0.9406 0.94055 0.005/0.11	0.9546 0.95470 -0.011/0.05	0.9647 0.96485 -0.016/0.04	0.9720 0.97236 -0.037/0.03	0.9778 0.97807 -0.027/0.10	0.9821 0.98248 -0.039/0.10
2.0265 (20)	0.8284 0.82774 0.080/0.10	0.8749 0.87564 -0.085/0.12	0.9066 0.90686 -0.029/0.07	0.9283 0.92856 -0.028/0.05	0.9438 0.94430 -0.052/0.03	0.9555 0.95607 -0.060/0.10	0.9645 0.96511 -0.063/0.10
3.0398 (30)		0.8030 0.80337 -0.046/0.13	0.8552 0.85607 -0.102/0.10	0.8904 0.89109 -0.078/0.06	0.9153 0.91586 -0.061/0.03	0.9334 0.93410 -0.075/0.10	0.9471 0.94794 -0.089/0.10
4.0530 (40)		0.7195 0.72034 -0.116/0.15	0.8013 0.80185 -0.068/0.15	0.8518 0.85248 -0.079/0.07	0.8866 0.88717 -0.064/0.04	0.9114 0.91227 -0.095/0.10	0.9302 0.93108 -0.095/0.10
5.0662 (50)		0.6190 0.61969 -0.112/0.16	0.7436 0.74369 -0.011/0.19	0.8124 0.81282 -0.052/0.08	0.8579 0.85839 -0.057/0.05	0.8898 0.89070 -0.101/0.10	0.9136 0.91463 -0.112/0.10
6.0795 (60)		0.4844 0.48496 -0.116/0.17	0.6818 0.68137 0.063/0.24	0.7723 0.77244 -0.018/0.11	0.8295 0.82977 -0.033/0.06	0.8688 0.86957 -0.088/0.10	0.8977 0.89869 -0.110/0.10
7.0928 (70)		0.3409 0.34062 0.083/0.18	0.6171 0.61595 0.186/0.28	0.7323 0.73196 0.047/0.14	0.8017 0.80167 0.003/0.07	0.8484 0.84909 -0.081/0.10	0.8825 0.88339 -0.101/0.10
8.1060 (80)		0.3170 0.31753 -0.165/0.20	0.5541 0.55235 0.317/0.32	0.6934 0.69253 0.125/0.15	0.7749 0.77458 0.042/0.09	0.8290 0.82951 -0.061/0.10	0.8682 0.86889 -0.079/0.10

9.1192	(90)	0.3273 0.32769 -0.120/0.22	0.5017 0.50134 0.071/0.35	0.6572 0.65598 0.185/0.17	0.7497 0.74911 0.079/0.11	0.8108 0.81112 -0.039/0.10	0.8548 0.85533 -0.062/0.10
10.133	(100)	0.3451 0.34535 -0.071/0.23	0.4706 0.47168 -0.230/0.38	0.6255 0.62461 0.142/0.18	0.7268 0.72601 0.109/0.12	0.7942 0.79423 -0.003/0.10	0.8425 0.84286 -0.043/0.10
11.146	(110)	0.3656 0.36574 -0.037/0.25	0.4605 0.46109 -0.129/0.41	0.6012 0.60048 0.120/0.20	0.7074 0.70602 0.196/0.13	0.7793 0.77915 0.019/0.10	0.8314 0.83165 -0.030/0.10
12.159	(120)	0.3872 0.38737 -0.043/0.27	0.4622 0.46272 -0.112/0.43	0.5847 0.58451 0.033/0.22	0.6913 0.68977 0.222/0.14	0.7665 0.76618 0.042/0.10	0.8218 0.82183 -0.003/0.10
13.172	(130)	0.4096 0.40961 -0.003/0.28	0.4711 0.47140 -0.063/0.46	0.5756 0.57626 -0.114/0.23	0.6793 0.67764 0.245/0.15	0.7559 0.75555 0.047/0.10	0.8136 0.81352 0.010/0.10
14.186	(140)	0.4321 0.43217 -0.016/0.30	0.4841 0.48418 -0.017/0.48	0.5731 0.57445 -0.236/0.24	0.6712 0.66968 0.226/0.15	0.7478 0.74739 0.055/0.10	0.8070 0.80681 0.024/0.10
15.199	(150)	0.4549 0.45488 0.005/0.32	0.4996 0.49946 0.029/0.50	0.5770 0.57765 -0.112/0.25	0.6668 0.66568 0.167/0.16	0.7421 0.74175 0.047/0.10	0.8020 0.80175 0.031/0.10
16.212	(160)	0.4777 0.47764 0.013/0.34	0.5166 0.51630 0.058/0.52	0.5839 0.58458 -0.116/0.25	0.6657 0.66522 0.072/0.16	0.7388 0.73858 0.030/0.10	0.7987 0.79836 0.043/0.10
17.225	(170)	0.5005 0.50040 0.021/0.36	0.5346 0.53416 0.082/0.54	0.5937 0.59426 -0.093/0.26	0.6679 0.66779 0.016/0.16	0.7379 0.73774 0.022/0.10	0.7969 0.79661 0.036/0.10
18.239	(180)	0.5233 0.52312 0.035/0.38	0.5533 0.55272 0.106/0.55	0.6055 0.60596 -0.076/0.28	0.6728 0.67290 -0.015/0.16	0.7391 0.73903 0.009/0.10	0.7969 0.79645 0.056/0.10
19.252	(190)	0.5460 0.54578 0.041/0.40	0.5724 0.57174 0.116/0.56	0.6188 0.61916 -0.058/0.28	0.6801 0.68010 0.000/0.16	0.7422 0.74225 -0.007/0.10	0.7980 0.79779 0.027/0.10
20.265	(200)	0.5687 0.56836 0.060/0.43	0.5906 0.59108 -0.081/0.57	0.6333 0.63348 -0.028/0.29	0.6889 0.68899 -0.014/0.15	0.7470 0.74716 -0.022/0.10	0.8007 0.80052 0.023/0.10
25.331	(250)	0.6798 0.67994 -0.020/0.48	0.6898 0.68993 -0.019/0.59	0.7149 0.71442 0.067/0.30	0.7494 0.74957 -0.022/0.14	0.7896 0.79006 -0.059/0.10	0.8309 0.83104 -0.017/0.10

30.398	(300)	0.7889 0.78919 -0.036/0.51	0.7888 0.78936 -0.071/0.61	0.8027 0.80186 0.105/0.30	0.8223 0.82345 -0.140/0.13	0.8503 0.85066 -0.043/0.10	0.8800 0.88026 -0.029/0.10
35.464	(350)	0.8962 0.89626 -0.006/0.55	0.8880 0.88791 0.010/0.63	0.8916 0.89095 0.073/0.30	0.9027 0.90231 0.043/0.11	0.9189 0.91925 -0.038/0.10	0.9390 0.93935 -0.037/0.10
40.530	(400)	1.0015 1.00137 0.013/0.57	0.9851 0.98520 -0.011/0.64	0.9802 0.98010 0.010/0.30	0.9839 0.98300 0.091/0.09	0.9913 0.99149 -0.019/0.10	1.0033 1.00359 -0.029/0.10
45.596	(450)	1.1046 1.10473 -0.011/0.58	1.0813 1.08118 0.011/0.65	1.0684 1.06871 -0.029/0.30	1.0653 1.06419 0.104/0.07	1.0652 1.06538 -0.017/0.10	1.0702 1.07052 -0.030/0.10
50.663	(500)	1.2063 1.20651 -0.018/0.58	1.1758 1.17587 -0.006/0.66	1.1560 1.15652 -0.045/0.30			
60.795	(600)	1.4058 1.40596 -0.011/0.58	1.3615 1.36171 -0.015/0.65	1.3293 1.32953 -0.018/0.28			
70.928	(700)	1.6008 1.60066 0.009/0.55	1.5430 1.54331 -0.020/0.64	1.4995 1.49909 0.028/0.25			
81.060	(800)	1.7920 1.79133 0.038/0.48	1.7208 1.72122 -0.025/0.62				

[dashed box] : the most probable value

1st line: skeleton table value, Z_{ST}

2nd line: calculated value, Z_{cal}

3rd line: deviation (%) / uncertainty (%)

(deviation = $[(Z_{ST} - Z_{cal}) / Z_{cal}] \times 100$)

Table 6 Calculated values of molar volume, molar enthalpy and molar entropy for gaseous ethane

Pressure MPa (atm)		Temperature K (°C)									
		273.15 (0)	298.15 (25)	323.15 (50)	348.15 (75)	373.15 (100)	398.15 (125)	423.15 (150)	448.15 (175)	473.15 (200)	498.15 (225)
0.101325	(1)	22185	24277	26360	28436	30507	32574	34639	36702	38763	40822
		-1354	-62	1306	2752	4276	5877	7556	9311	11143	13049
		-4.53	0.00	4.41	8.71	12.94	17.09	21.18	25.21	29.18	33.11
1.0133	(10)	1993.7	2248.6	2489.5	2721.6	2947.7	3169.8	3388.7	3605.4	3820.3	4033.8
		-2101	-656	819	2342	3925	5573	7289	9075	10932	12859
		-25.61	-20.55	-15.80	-11.26	-6.87	-2.60	1.58	5.68	9.71	13.68
2.0265	(20)	840.09	1010.7	1156.3	1289.4	1414.9	1535.4	1652.5	1767.0	1879.6	1990.8
		-3165	-1424	219	1853	3515	5222	6984	8807	10694	12646
		-34.30	-28.19	-22.90	-18.03	-13.42	-8.99	-4.70	-0.51	3.58	7.60
3.0398	(30)		580.68	705.12	808.91	902.58	990.18	1073.8	1154.5	1233.2	1310.3
			-2398	-468	1319	3079	4856	6670	8533	10453	12432
			-34.07	-27.85	-22.52	-17.64	-13.03	-8.61	-4.34	-0.17	3.91
4.0530	(40)		328.89	471.96	565.99	645.42	717.31	784.54	848.62	910.45	970.59
			-3974	-1290	728	2615	4474	6347	8254	10208	12216
			-40.89	-32.21	-26.19	-20.95	-16.13	-11.57	-7.19	-2.95	1.19
5.0662	(50)			321.78	417.70	490.40	553.51	611.21	665.43	717.21	767.22
				-2361	63	2118	4075	6015	7971	9962	11998
				-36.75	-29.51	-23.81	-18.73	-14.01	-9.52	-5.20	-1.00
6.0795	(60)			204.82	316.61	386.62	444.42	495.97	543.69	588.82	632.07
				-4027	-698	1585	3660	5674	7683	9713	11781
				-42.73	-32.76	-26.42	-21.04	-16.13	-11.52	-7.11	-2.85
7.0928	(70)				243.19	312.50	366.80	414.06	457.16	497.53	535.95
					-1574	1017	3230	5327	7392	9464	11564
					-36.09	-28.89	-23.14	-18.04	-13.29	-8.80	-4.47
8.1060	(80)				189.79	257.54	309.14	353.12	392.73	429.49	464.26
					-2533	419	2789	4975	7100	9215	11347
					-39.46	-31.26	-25.11	-19.78	-14.90	-10.31	-5.92
9.1192	(90)				153.93	216.21	265.08	306.32	343.11	377.01	408.89
					-3438	-190	2342	4622	6808	8967	11133
					-42.56	-33.53	-26.96	-21.40	-16.38	-11.70	-7.24
10.133	(100)				131.95	185.30	230.86	269.57	303.94	335.46	364.98
					-4158	-779	1899	4271	6519	8722	10921
					-45.04	-35.66	-28.70	-22.92	-17.76	-12.98	-8.44

11.146	(110)	162.49 -1318 -37.57	204.07 1471 -30.33	240.24 3927 -24.34	272.43 6235 -19.04	301.89 8481 -14.17	329.41 10713 -9.57
12.159	(120)	145.78 -1787 -39.24	183.01 1067 -31.83	216.57 3596 -25.67	246.73 5958 -20.25	274.35 8246 -15.28	300.12 10510 -10.62
13.172	(130)	133.47 -2181 -40.68	166.39 697 -33.21	197.32 3280 -26.91	225.52 5691 -21.38	251.46 8017 -16.32	275.68 10312 -11.60
14.186	(140)	124.26 -2508 -41.90	153.21 363 -34.45	181.54 2984 -28.07	207.86 5435 -22.44	232.23 7797 -17.31	255.04 10120 -12.52
15.199	(150)	117.22 -2776 -42.95	142.67 67 -35.57	168.53 2710 -29.13	193.03 5194 -23.43	215.94 7586 -18.23	237.45 9935 -13.40
16.212	(160)	111.72 -2997 -43.85	134.16 -193 -36.58	157.72 2458 -30.12	180.50 4966 -24.36	202.03 7384 -19.11	222.34 9757 -14.22
17.225	(170)	107.33 -3180 -44.64	127.22 -420 -37.48	148.68 2229 -31.03	169.84 4754 -25.23	190.06 7194 -19.93	209.26 9587 -15.00
18.239	(180)	103.73 -3331 -45.33	121.48 -618 -38.29	141.05 2022 -31.86	160.71 4557 -26.04	179.71 7014 -20.70	197.87 9426 -15.74
19.252	(190)	100.74 -3457 -45.95	116.69 -790 -39.03	134.57 1835 -32.63	152.84 4375 -26.80	170.70 6845 -21.44	187.88 9272 -16.44
20.265	(200)		112.63 -939 -39.69	129.02 1667 -33.34	146.02 4208 -27.51	162.81 6687 -22.13	179.08 9127 -17.10
25.331	(250)			110.36 1060 -36.20	122.50 3562 -30.46	135.04 6049 -25.06	147.59 8521 -19.96
30.398	(300)				109.00 3162 -32.65	118.68 5621 -27.31	128.61 8091 -22.23

1st line: molar volume V in $cm^3 \cdot mol^{-1}$

2nd line: molar enthalpy H in $J \cdot mol^{-1}$

3rd line: molar entropy S in $J \cdot K^{-1} mol^{-1}$

Table 7 Calculated values of molar volume, molar enthalpy and molar entropy for gaseous ethene

Pressure MPa	(atm)	Temperature K (°C) 273.15 (0)	298.15 (25)	323.15 (50)	348.15 (75)	373.15 (100)	398.15 (125)	423.15 (150)
0.101325	(1)	22244	24325	26399	28469	30536	32599	34661
		-1109	-45	1034	2278	3536	4855	6236
		-3.73	0.00	3.64	7.19	10.68	14.10	17.47
1.0133	(10)	2062.1	2301.1	2531.5	2756.4	2977.3	3195.4	3411.4
		-1632	-473	725	1971	3269	4621	6028
		-24.20	-20.14	-16.28	-12.57	-8.97	-5.47	-2.04
2.0265	(20)	927.64	1071.1	1202.4	1326.4	1445.7	1561.8	1675.5
		-2312	-1000	297	1612	2962	4355	5794
		-31.77	-27.17	-22.99	-19.07	-15.33	-11.71	-8.21
3.0398	(30)		655.15	756.67	848.56	934.77	1017.3	1097.2
			-1602	-169	1233	2644	4081	5555
			-32.03	-27.41	-23.23	-19.32	-15.59	-12.00
4.0530	(40)		440.58	531.56	608.84	679.12	745.12	808.24
			-2319	-682	830.2	2312	3800	5313
			-36.26	-30.98	-26.48	-22.37	-18.51	-14.82
5.0662	(50)		303.22	394.40	464.42	525.67	582.00	635.16
			-3239	-1255	402	1968	3513	5067
			-40.60	-34.19	-29.25	-24.91	-20.90	-17.11
6.0795	(60)		197.75	301.1[illegible]	367.79	423.45	473.49	520.08
			-4620	-1904	-55	1611	3220	4819
			-46.08	-37.28	-31.77	-27.14	-22.97	-19.08
7.0928	(70)		119.05	233.33	298.72	350.67	396.29	438.19
			-6682	-2644	-539	1243	2922	4569
			-53.51	-40.41	-34.12	-29.18	-24.82	-20.81
8.1060	(80)		97.104	183.08	247.30	296.46	338.76	377.12
			-7623	-3463	-1048	866.2	2620	4317
			-57.03	-43.59	-36.38	-31.06	-26.51	-22.38
9.1192	(90)		89.079	147.71	208.22	254.86	294.44	329.99
			-8029	-4278	-1570	484	2318	4067
			-58.71	-46.63	-38.53	-32.83	-28.07	-23.81
10.133	(100)		84.490	125.07	178.44	222.30	259.48	292.66
			-8272	-4963	-2085	103[illegible]	2016	3818
			-59.82	-49.17	-40.58	-34.50	-29.53	-25.15
11.146	(110)		81.344	111.15	155.95	196.53	231.41	262.52
			-8439	-5473	-2570	-270	1719	3572
			-60.66	-51.12	-42.45	-36.07	-30.90	-26.39
12.159	(120)		78.975	102.25	139.15	176.00	208.60	237.80
			-8563	-5843	-3003	-627	1430	3332
			-61.34	-52.60	-44.13	-37.53	-32.19	-27.55
13.172	(130)		77.087	96.153	126.64	159.61	189.88	217.29
			-8658	-6117	-3376	-961	1152	3099
			-61.93	-53.76	-45.58	-38.88	-33.39	-28.65
14.186	(140)		75.523	91.707	117.22	146.47	174.41	200.10
			-8733	-6326	-3689	-1266	888	2874
			-62.44	-54.70	-46.84	-40.11	-34.52	-29.68
15.199	(150)		74.191	88.293	110.02	135.89	161.56	185.59
			-8793	-6490	-3950	-1541	641	2660
			-62.89	-55.49	-47.92	-41.23	-35.57	-30.65
16.212	(160)		73.035	85.566	104.38	127.30	150.81	173.26
			-8841	-6622	-4167	-1784	412	2456
			-63.31	-56.17	-48.85	-42.24	-36.54	-31.56
17.225	(170)		72.014	83.319	99.863	120.28	141.78	162.71
			-8881	-6729	-4349	-1999	202	2265
			-63.69	-56.76	-49.67	-43.15	-37.44	-32.41

18.239	(180)	71.101	81.423	96.172	114.47	134.14	153.64
		-8913	-6818	-4502	-2188	10	2086
		-64.04	-57.30	-50.39	-43.97	-38.27	-33.21
19.252	(190)	70.276	79.792	93.096	109.60	127.63	145.79
		-8939	-6892	-4631	-2353	-164	1919
		-64.36	-57.78	-51.04	-44.72	-39.04	-33.97
20.265	(200)	69.525	78.367	90.487	105.48	122.05	138.98
		-8959	-6955	-4742	-2498	-322	1765
		-64.67	-58.22	-51.63	-45.40	-39.75	-34.67
25.331	(250)	66.539	73.179	81.638	91.805	103.25	115.42
		-9007	-7149	-5103	-2997	-900	1164
		-65.98	-60.01	-53.91	-48.07	-42.63	-37.60
30.398	(300)	64.359	69.771	76.358	84.046	92.640	101.88
		-8993	-7226	-5279	-3265	-1237	784
		-67.05	-61.36	-55.56	-49.98	-44.72	-39.79
35.464	(350)	62.649	67.270	72.722	78.938	85.808	93.190
		-8942	-7239	-5357	-3406	-1431	550
		-67.96	-62.48	-56.87	-51.46	-46.34	-41.51
40.530	(400)	61.247	65.311	69.999	75.248	80.982	87.118
		-8867	-7211	-5376	-3469	-1535	414
		-68.76	-63.43	-57.96	-52.67	-47.66	-42.91
45.596	(450)	60.061	63.709	67.846	72.411	77.349	82.602
		-8774	-7155	-5355	-3482	-1578	344
		-69.48	-64.27	-58.90	-53.71	-48.77	-44.09
50.663	(500)	59.035	62.360	66.079			
		-8668	-7079	-5306			
		-70.13	-65.32	-59.74			
55.729	(550)	58.133	61.198	64.588			
		-8551	-6988	-5237			
		-70.73	-65.70	-60.49			
60.795	(600)	57.329	60.180	63.304			
		-8427	-6884	-5152			
		-71.30	-66.34	-61.17			
65.861	(650)	56.603	59.275	62.179			
		-8295	-6771	-5054			
		-71.83	-66.92	-61.81			
70.928	(700)	55.944	58.462	61.180			
		-8159	-6651	-4946			
		-72.32	-67.47	-62.39			
75.994	(750)	55.339	57.725				
		-8018	-6524				
		-72.80	-67.99				
81.060	(800)	54.782	57.051				
		-7873	-6391				
		-73.25	-68.48				

1st line: molar volume V in $cm^3 \cdot mol^{-1}$

2nd line: molar enthalpy H in $J \cdot mol^{-1}$

3rd line: molar entropy S in $J \cdot K^{-1} mol^{-1}$