BULLETIN OF THE CHEMICAL SOCIETY OF JAPAN VOL. 42 3415—3421 (1969)

Thermodynamic Properties of Carbon Tetrafluoride from 4°K to Its Melting Point[*1]

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(Received May 22, 1969)

Thermodynamic properties of solid and liquid carbon tetrafluoride were measured at temperatures from 4°K to 100°K. The heat of transition was found to be 349.5 ± 0.9 cal/mol, the transition temperature 76.221°K, the heat of fusion 168.6 ± 0.05 cal/mol, the triple point temperature 89.515°K and the triple point pressure 0.80 ± 0.03 Torr. The amount of impurity in the specimen of CF_4 was estimated to be 0.014_7 mol% from the measurement of the melting point range. The values of molal entropy of CF_4 as an ideal gas at 298.2°K, were calculated from the calorimetric and spectroscopic data as 62.63 e.u. and 62.45 e.u., respectively. The Debye characteristic temperature at 0°K was derived from the low temperature heat capacity data, and the $\theta_D(T)$ curve was compared with that for neopentane taking into account the octupole interaction of molecules in the crystal.

Carbon tetrafluoride CF_4 is one of a few tetrahedral molecules which undergo phase transition in solid state. The measurements of heat capacity were made by Eucken and Schröder in the region from 12°K to its boiling point,[1)] and by Kostryukov *et al.* in the region from 12—13°K to its melting point.[2)] The vapor pressure was measured by Menzel and Mohry in solid and liquid states.[3)]

The purpose of this paper is to provide more complete and accurate data on the thermodynamic properties of CF_4 from 4°K to its melting point and give a theoretical consideration on the vibrational property of the molecule at low temperature. The data are compared with those of others. A comparison of the entropy calculated from calorimetric data with spectroscopic data is made based on the third low of thermodynamics.

The Debye characteristic temperature, $\theta_D(T)$, is derived from the low temperature heat capacity data, and a comparison of the temperature dependence of $\theta_D(T)$ below 15°K is made with these for other molecular crystals reported by the present authors on a reduced scale using the Debye characteristic temperature at 0°K, $\theta_D(0)$.

Experimental

Material. Chemically pure CF_4 obtained from the Matheson Co., was found to contain about 2.2% of air. This was purified before introduction into the calorimeter vessel. The gas was passed through a 3N KOH solution to remove impurities such as CO_2, SiF_4, SO_2, F_2, and then through a tube containing $CaCl_2$. The resulting material was distilled three times, at liquid nitrogen temperature, through pyrex glass fractionating bulb in a vacuum. The middle fraction collected was cooled to liquid nitrogen temperature and pumping was carried out for two days at a pressure less than 10^{-3} Torr in order to remove the trace of air from the sample. The mole numbers of actual specimen were measured by using a calibrated bulb attached to the calorimeter filling system, and then condensed into the calorimeter vessel. As grease of cock, 'Phynal' was employed instead of silicone grease. No impurity of the sample was found from gas chromatography using a Shimadzu Gas Chromatograph GC-1C. The amount of solid-insoluble liquid-soluble impurity found from measurement of the melting point was 0.014_7 mol%.

Apparatus. The cryostat, experimental techniques and temperature scale were the same as those used in the measurement of $C(CH_3)_4$.[4)] A new calorimeter vessel made of silver-plated copper (0.2 mm thick, internal volume about 45 cm^3) was employed.

Results

Heat Capacity of CF_4. The calorimeter contained 0.21789 mol of the sample in measurement series I, 0.34522 mol in series II and 0.33264 mol in series III. Samples in series I, II and III were taken from separate fillings from the same sample. The heat capacity data are given in Table 1. Correction was necessary above 80°K for vaporization of CF_4 which occurred during the measure-

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[*1] Presented at the 22nd Annual Meeting of the Chemical Society of Japan, Tokyo, April, 1969.

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1) A. Eucken and E. Schröder, *Z. Pkysik. Chem.*, **B41**, 307 (1938).

2) V. N. Kostryukov, O. P. Samorukov and P. Strelkov, *Zhur. Fiz. Khim.*, **32**, 1354 (1958).

3) W. Menzel and F. Mohry, *Z. Anorg. Allgem. Chem.*, **210**, 257 (1933).

4) H. Enokido, T. Shinoda and Y. Mashiko, This Bulletin, **42**, 84 (1969).

ment. For values of heat of vaporization and of heat capacity of gaseous CF_4 those obtained by Eucken and Schröder1) and Hwang and Martin5) were used. The volume of the sample condensed in the calorimeter vessel was calculated using densities of solid and liquid CF_4 given by Stewart and Rock6) and Knobler and Pings7). Gas imperfection correction was negligible over the termperature range of measurement. Correction was made with respect to curvature where necessary. The heat capacity data are plotted in Fig. 1 along with those given by Eucken and Schröder.1) The results agree in the terperature range from 12 to 55°K. However, above 60°K, in particular between transition point and melting point, a difference is seen. The heat capacity of solid CF_4 between 12—13°K and the melting point was measured by Kostryukov *et al.*2) The results were given graphically, but numerical values were not reported. A comparison of the result of Kostryukov *et al.* with ours from the heat capacity curve for CF_4 in Fig. 4 of Ref. 2 may be regarded as in good agreement.

TABLE 1. HEAT CAPACITY OF CF_4
(Molecular weight 88.005; 1cal=4.1840 absolute joules; 0°C=273.15°K)

T (°K)	C_p (cal/deg mol)	T (°K)	C_p (cal/deg mol)
4.024	0.05130	27.648	7.360
4.039	0.05202	29.039	7.735
4.432	0.07149	53.130	12.63
4.458	0.07149	55.192	13.06
4.897	0.09829	57.132	13.43
4.931	0.09901	59.035	13.82
5.151	0.1148	60.906	14.23
5.423	0.1372	62.715	14.66
5.497	0.1432	64.465	15.12
5.648	0.1603	66.050	15.54
5.774	0.1716	67.482	15.96
6.140	0.2142	68.871	16.45
6.237	0.2244	70.143	17.03
6.643	0.2723	71.291	17.66
6.669	0.2780	72.332	18.28
7.109	0.3503	73.188	18.85
7.140	0.3499	73.920	19.52
7.612	0.4416	74.597	20.06
7.640	0.4386	74.702	20.18
8.120	0.5413	75.247	20.62
8.141	0.5434	75.265	20.88
8.619	0.6615	75.257	20.92
8.642	0.6633	75.609	21.77
9.128	0.8004	75.741	22.24
9.148	0.8025	75.891	22.64
9.646	0.9182	75.908	22.74
9.663	0.9219	76.221	‘Transition’
10.163	1.129	76.611	15.78
10.334	1.205	76.656	15.77
10.824	1.376	77.104	15.86
10.830	1.396	80.312	16.14
11.412	1.613	81.416	16.23
11.622	1.688	82.241	16.31
13.536	2.413	82.344	16.33
14.206	2.686	83.237	16.40
14.643	2.892	83.180	16.41
15.233	3.110	84.223	16.47
15.605	3.277	84.229	16.48
16.282	3.517	85.256	16.56
16.587	3.656	85.397	16.58
17.346	3.924	86.286	16.66
17.579	4.027	86.536	16.69
18.677	4.413	87.282	16.74
19.891	4.811	87.673	16.80
21.147	5.324	88.314	16.88
22.374	5.726	88.720	16.96
23.601	6.133	89.515	‘Fusion’
25.017	6.596	90.389	18.70
26.305	6.982	91.716	18.79

The transition seemed to be first-order at the start, but changed into second-order type gradually after passing the middle point of the process and finished as the second-order one. This situation is different from that in $C(CH_3)_4$ crystal reported previously which seemed to be second-order over the whole transition range. We observed this heat capacity anomaly to have a very large value (*i.e.* 61.31 cal/mol deg at 76.336°K). No hysteresis was observed.

TABLE 2. TRANSITION AND TRIPLE POINT OF CF_4
“Transtion point”

Fraction transformed	T (°K)
0.19860	76.211
0.50859	76.218
0.98805	76.221
$T_{\text{transition}}$	76.221
Eucken and Schröder (1938)	76.23
Kostryukov, Samorukov and Strelkov (1958)	76.09±0.012

“Triple point”

Fraction melted	T (°K)	P (Torr)
0.17018	89.449	0.80
0.23510	89.468	0.83
0.32558	89.485	0.80
0.50641	89.503	0.78
		average 0.80±0.03
T_{triple} (pure CF_4)	89.529	
Eucken *et al.* (1938)	89.47	
Kostryukov *et al.* (1958)	88.44±0.02	

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5) Y. Hwang and J. J. Martin, *A. I. Ch. E. J.*, **10**, 89 (1964).

6) J. W. Stewart and R. I. L. Rock, *J. Chem. Phys.*, **28**, 425 (1958).

7) C. M. Knobler and C. J. Pings, *J. Chem. Eng. Data*, **10**, 129 (1965).

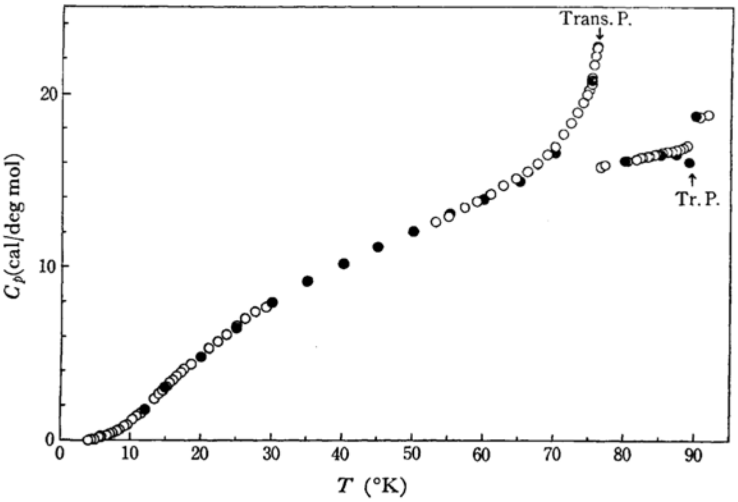

Fig. 1. Heat capacity curve of CF_4.
●: Eucken *et al.* ○: Present research

The Transition and the Triple Points. The transition temperature was determined from percentages of the specimen transformed and the measured equilibrium termperatures using the first-order law. The result is summarized in Table 2.

The triple point temperature corresponding to pure CF_4 was obtained from a plot of the equilibrium temperatures against the reciprocals of the fraction melted, and the result is given in Table 2 together with the triple point pressures. The triple point temperatures for pure CF_4 and the sample used are found to be 89.529°K and 89.515°K, and the values are compared with those given by others in Table 2.

Heat of Transition and Fusion. Data of the heat of transition and fusion are summarized in Table 3 together with those given by others. Our results are in good agreement with those of Eucken and Schröder, but not with Kostryukov *et al.*, particularly in that of the heat of transition which deviates considerably from ours. In the present measurement the average deviation of the result of the heat of transition is larger than that of the heat of fusion. This is probably due to the fact that a $\int C_p \mathrm{d}T$ correction at temperatures slightly above the transition point was not estimated exactly, because the end of transition is a second-order type.

The Vapor Pressure Measurements. The vapor pressure of CF_4 was measured at temperatures

Table 3. Heat of transition and fusion of CF_4

Temperature interval (°K)	Heat input (cal/mol)	$\int C_p \mathrm{d}T$ (cal/mol)	ΔH (cal/mol)
	"Transition" (mol wt 88.005; (i) 0.21789 mol, (ii) 0.21789 mol)		
(i) 75.952—76.270	367.3	16.9	350.4
(ii) 76.078—76.639	369.6	21.0	348.6
		average	349.5±0.9
Eucken and Schröder (1938)			354.0 352.5
Kostryukov *et al.* (1958) 74.4—76.0	414.5	47.8	366.7
	"Fusion" ((i) 0.21789 mol, (ii) 0.34522 mol)		
(i) 89.057—89.620	187.3	18.8	168.5
(ii) 89.237—89.556	177.4	8.8	168.6
		average	169.6±0.05
Eucken and Schröder (1938)			167.0 167.7
Kostryukov *et al.* (1958)			165.8

from 80 to 102°K, and is listed in Table 4. The result was made to fit the following equations by the method of least squares:

i) $80°\text{K} < T <$ triple point

$$\log_{10}P + 2(\log_{10}T) = 19.1433 - (1363.87)/T, \qquad (1)$$

ii) $T >$ triple point

$$\log_{10}P + 2(\log_{10}T) = 14.0430 - (920.65)/T. \qquad (2)$$

The deviation of the observed values from those calculated by means of Eqs. (1) and (2) are given in the last column of Table 4, and are plotted by open circles in Fig. 2.

TABLE 4. VAPOR PRESSURE OF SOLID AND LIQUID CF_4

T (°K)	$P_{\text{obs.}}$ (Torr)	$P_{\text{obs.}} - P_{\text{calc.}}$ (Torr)
Solid		
80.878	0.036	+0.007
81.952	0.066	+0.019
82.734	0.021	−0.046
83.625	0.110	+0.012
84.823	0.206	+0.045
85.968	0.349	+0.092
87.104	0.528	+0.125
88.236	0.605	−0.019
89.204	0.784	−0.114
89.346	0.798	−0.149
Liquid		
89.713	0.708	−0.042
91.057	1.009	−0.023
92.361	1.421	+0.028
93.641	1.977	+0.122
94.917	2.587	+0.139
96.012	3.290	+0.204
97.703	4.468	+0.102
99.679	6.267	−0.185
101.464	8.369	−0.682

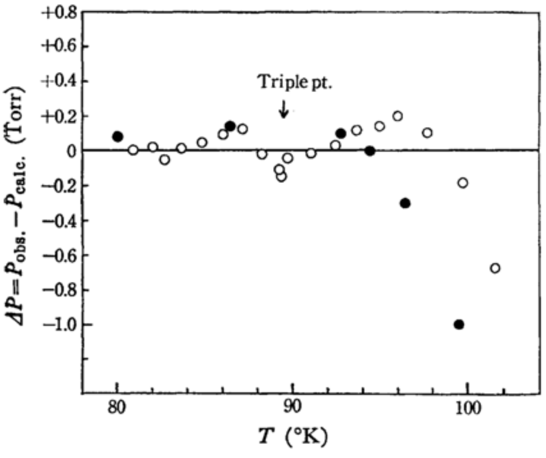

Fig. 2. Deviation of observed vapor pressure of CF_4 from the calculated one by using Eqs. (1) and (2).
●: Menzel and Mohry ○: Present research

In Fig. 2 are shown also the deviations between the pressures observed by Menzel and Mohry[3] and those calculated. Over a large part of the temperature region of measurement these differences are considerably large, since the absolute values of pressure are very small.

Entropy. The calorimetric and spectroscopic entropies of the ideal gaseous CF_4 at 298.2°K were calculated and compared with those obtained by Eucken and Schröder as shown in Table 5. The entropy below 4°K was estimated by using the value of Debye characteristic temperature obtained from the extrapolation of plots of $\theta_D(T)$ *versus* T. As the entropy of the vaporization and that above 122°K the values given by Eucken and Schröder were used.

As the entropy obtained by Eucken and Schörder is largely different from ours between 12°K and the transition point even taking into account probale errors in both measurements, we re-calculated the value using the heat capacity data observed by them. The value obtained is not 15.26 e.u. but 15.56 e.u. and agrees with ours within accuracy of their measurement. Therefore, the calorimetric entropy

TABLE 5. THE ENTROPY OF CF_4 GAS AT 298.2°K

	Eucken and Schröder (e. u.)	Present research (e. u.)
" Calorimetric "		
0—12°K	0.69	0.60
12°K-Transition	15.26(15.56)	15.61
Transition	4.64	4.59
Transition-Fusion	2.59	2.63
Fusion	1.87	1.88
Fusion-122°K	5.81	5.77
Vaporization	25.55	25.55
122—298.2°K	9.96	9.96
Compression from 0.1365 to 1 atm	−3.94	−3.96
	62.43(62.73)	62.63
" Spectroscopic "		
Translational	—	39.34
Rotational	—	20.00
Vibrational	—	3.11
Total	62.81	62.45
Moment of inertia I (10^{-40} g cm^2)	101.3	145.9*3
Vibrational frequencies (cm^{-1})	899 435 1343 650	904[8] 437 1265 630

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*3 This is the value calculated using atomic distances obtained by Hoffman and Livingston (*J. Chem. Phys.*, **21**, 565 (1953)) from their measurements of electron diffraction.

8) D. M. Yost, E. N. Lassettre and S. T. Gross, *J. Chem. Phys.*, **4**, 325 (1936).

obtained by these authors is to be estimated as 62.73 e.u. On the other hand, the difference of the spectroscopic entropy may arise from the discrepancy of the values of the moment of inertia and the vibrational frequencies used in calculations as listed in Table 5. Agreement of the calorimetric entropy of 62.63 e.u. and the spectroscopic entropy of 62.45 e.u. is satisfactory as is seen in Table 5.

Discussion

In order to elucidate lattice vibrations at low temperature, we converted the observed heat capacity data of CF_4 and $C(CH_3)_4$ to the Debye characteristic temperature, $\theta_D(T)$, assuming $6N$ degrees of vibrational freedom (where N is Avogadro's number). Here, $C_p - C_v$ correction was neglected, since little is known about the thermal expansion and compressibility of CF_4 and $C(CH_3)_4$ crystals. We can neglect this term, since the contribution to $\theta_D(T)$ will be small at low temperature. However, the contribution of the intramolecular vibrations to the heat capacity was taken into account using the observed infrared and Raman spectral data.[8] In order to compare the temperature dependence of the $\theta_D(T)$ for CF_4 with that for $C(CH_3)_4$, the values of $\theta_D(T)$ were plotted against temperature on a reduced scale using the Debye characteristic temperature at 0°K, $\theta_D(0)$, as shown in Fig. 3. Here the intramolecular rotational frequency of the methyl group in $C(CH_3)_4$ of 286 cm^{-1} obtained by Rush[9] from his cold-neutron study was used. The values of $\theta_D(0)$ for CF_4 and $C(CH_3)_4$ were calculated from the first coefficients of the expansion of low temperature heat capacity, *i.e.*

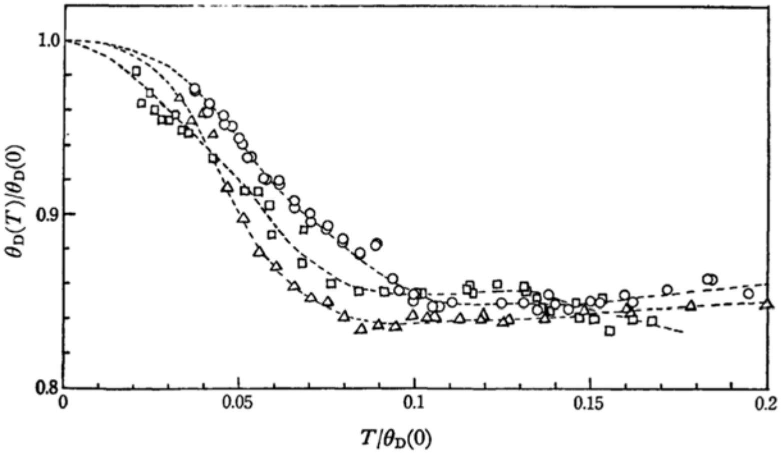

Fig. 3. $\theta_D(T)$ curves on a reduced basis.
○: CF_4 △: $C(CH_3)_4$ □: CO

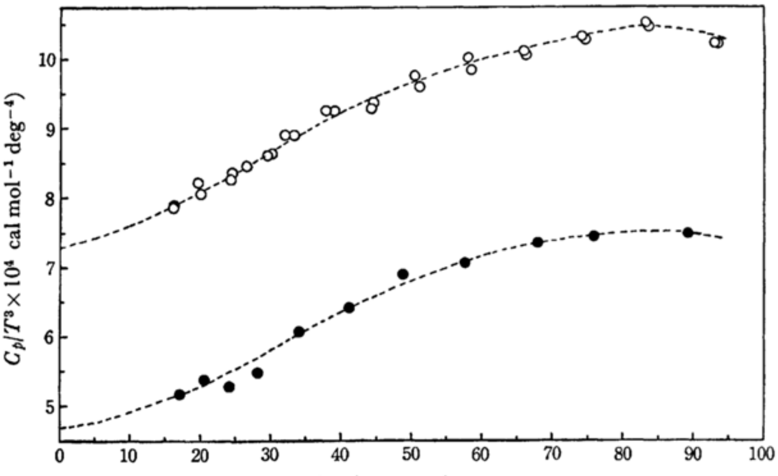

Fig. 4. Plots of C_p/T^3 against T^2 for CF_4 and $C(CH_3)_4$.
○: CF_4 ●: $C(CH_3)_4$

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[9] J. J. Rush, *J. Chem. Phys.*, **46**, 2285 (1967).

TABLE 6. THE VALUES OF POTENTIAL PARAMETERS FOR CF_4, $C(CH_3)_4$ AND CO

		CF_4	$C(CH_3)_4$	CO
Lennard-Jones parameters[a)]	ε/k (°K)	141	191	88
	r_0 (A)	4.63	6.44	3.706
Anisotropy factor[b)]	κ	0	0.0528	0.0905
Polarizability[c)]	α (A^3)	2.89	10.07	1.844
Quadrupole moment[d)]	$\sum_i e_i(z_i^2-x_i^2)$(esu)	—	—	$0.92—2.81\times10^{-26}$
Octupole moment[e)]	$\sum_i e_i x_i y_i z_i$(esu)	4.44×10^{-24}	25.2×10^{-34}	—

a) J. C. McCoubrey and N. M. Singh, *Tranns. Faraday Soc.*, **53**, 877 (1957).
b) C. Clement and P. Bothorel, *J. Chim. Phys.* **61**, 878 (1964).
c) W. Brandt, *J. Chem. Phys.*, **24**, 501 (1956).
d) R. H. Orcutt, *ibid.*, **39**, 605 (1963).
e) The octupole moment of 5.48×10^{-34} esu for CF_4 has recently been estimated by Spurling *et al.* (*J. Chem. Phys.*, **48**, 1006 (1968)) in the same way as ours. Also from their measurements of far-infrared absorption in gaseous CF_4 Rosenberg *et al.* (*J. Chem. Phys.*, **48**, 1396 (1968)) obtained the octupole moment for CF_4 of 4.5 or 4.8×10^{-34} esu.

$$\theta_D(0) = (935.14/\boldsymbol{\alpha})^{1/3}, \tag{3}$$

where $\boldsymbol{\alpha}$ has the unit of $cal\cdot mol^{-1}\cdot deg^{-4}$. The values of $\boldsymbol{\alpha}$ obtained from plots of C_p/T^3 against T^2 as given in Fig. 4 correspond to $\theta_D(0)=108.7°$ for CF_4 and $\theta_D(0)=125.9°$ for $C(CH_3)_4$.

In higher temperature region above $T/\theta_D(0)=0.1$, it is difficult to obtain information on lattice vibrations in solid CF_4 and $C(CH_3)_4$ from the $\theta_D(T)/\theta_D(0)$ curves, since in this region C_p-C_v correction and anharmonicity in lattice vibrations must be taken into consideration. At low temperature region below $T/\theta_D(0)=0.1$, however, difference in the shapes of the $\theta_D(T)/\theta_D(0)$ curves for CF_4 and $C(CH_3)_4$ shown in Fig. 3 may be accounted for by the interaction between molecular octupoles which plays the most important part in lattice vibrations of tetrahedral molecules.[*4] The values of octupole moment for CF_4 and $C(CH_3)_4$ was estimated using the second virial coefficient data. The analysis is given in Appendix, and the values obtained are listed in Table 6 together with the other potential parameters. The octupole moment for CF_4 is smaller than that for $C(CH_3)_4$. Treatment on the basis of lattice theory already made for CO crystal[10)] will give us insight into the molecular motions at low temperature of CF_4 and $C(CH_3)_4$. For comparison, the $\theta_D(T)/\theta_D(0)$ curve and the values of the potential parameters of molecular interactions for CO are given in Fig. 3 and Table 6, where multipole is quadrupole.

Data of the thermodynamic properties for CF_4 reported in this paper provide the first observed values in the temperature range below 12°K. The values are complete and more accurate than have been available heretofore in the temperature range above 12°K.

The authors are grateful to Mr. Ichiro Takeda of the Government Chemical Industrial Research Institute, Tokyo for help in measurement of gas chromatography.

Appendix

The second virial coefficient $\boldsymbol{B}$ for a tetrahedral molecule has been given by Kielich[11)] as follows:

$$\begin{aligned}\boldsymbol{B} = (2/3)\pi \boldsymbol{N} r_0^3[F(y) &- \kappa^2(0.050+0.095\kappa^2)H_{12}(y) \\ &- (3/5y^2)(\alpha/r_0^3)(\Omega^2/\varepsilon r_0^7)H_{10}(y) \\ &- (297/350)\Omega^2/\varepsilon r_0^7)^2 H_{14}(y)],\end{aligned} \tag{4}$$

where the first term represents the contribution of a Lennard-Jones 6-12 potential, the second the effect of anisotropy on the dispersion forces, the third from the interaction of an induced dipole with the octupole and the fourth the inetraction between octupole moments. Here ε and r_0 are the Lennard-Jones potential parameters, α is the polarizability of the molecule, Ω is its anisotropy and Ω is defined by the octupole moment $\sum_i e_i x_i y_i z_i$ as

$$\Omega = (5/2)\sum_i e_i x_i y_i z_i \tag{5}$$

for a tetrahedral molecule.

The function $F(y)$ is tabulated by Hirschfelder *et al.*[12)] with $y=2(\boldsymbol{k}T/\varepsilon)^2$, and the function $H_n(y)$ is tabulated by Buckingham and Pople.[13)] By using known values of ε, r_0, α, and κ, the value of the octupole moment was

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[*4] Although information on the effect of the octupole interaction on lattice vibrations for tetrahedral molecules has not yet been given, the phase transitions in solid methane have been successfully explained by the octupole interaction. Some typical reference may be quoted here; H. M. James and T. A. Keenan, *J. Chem. Phys.*, **31**, 12 (1959); T. Yamamoto, *ibid.*, **48**, 3193 (1968); T. Yamamoto and Y. Kataoka, *ibid.*, **48**, 3199 (1968).

10) T. Shinoda and H. Enokido, *J. Phys. Soc. Japan*, **26**, 1353 (1969).

11) S. Kielich, *Physica*, **31**, 444 (1965).

12) J. O. Hirschfelder, C. F. Curtiss and R. B. Bird, "Molecular Theory of Gases and Liquids," John Wiley & Sons, Inc., New York (1954), p. 1114.

13) A. D. Buckingham and J. A. Pople, *Trans. Faraday Soc.*, **51**, 1173 (1955).

TABLE 7. CALCULATED AND EXPERIMENTAL SECOND VIRIAL COEFFICIENTS (in units of $cm^3 mol^{-1}$)

" Carbon tetrafluoride "

T (°K)	B_{L-J}	$B_{O-ind\mu}$	B_{O-O}	B_{calc}	B_{obs}[a)]
273.16	−85.2	−2.6	−20.4	−108.2	−111.0
294.16	−70.3	−2.4	−17.7	−90.4	−101.0
298.153	−67.7	−2.4	−17.2	−87.3	−88.30
303.152	−64.6	−2.3	−16.6	−83.5	−84.40
313.16	−58.7	−2.2	−15.7	−76.6	−83.6
323.16	−42.5	−2.2	−14.8	−59.5	−72.4
323.16	−42.5	−2.2	−14.8	−59.5	−70.4
348.153	−41.1	−2.0	−12.9	−56.0	−55.70
348.16	−41.1	−2.0	−12.8	−55.9	−56.1
373.16	−30.8	−1.9	−11.3	−44.0	−43.50
373.16	−30.8	−1.9	−11.3	−44.0	−43.9
373.16	−30.8	−1.9	−11.4	−44.1	−43.1
398.16	−22.0	−1.8	−10.1	−33.9	−30.1
398.16	−22.0	−1.8	−10.1	−33.9	−33.20
398.16	−22.0	−1.8	−10.1	−33.9	−31.1
423.16	−14.4	−1.7	−9.1	−25.2	−26.0
423.183	−14.4	−1.7	−9.1	−25.2	−24.40
448.197	−7.7	−1.6	−8.2	−17.5	−16.80
473.213	−1.9	−1.5	−7.5	−10.9	−10.10
498.229	+3.3	−1.4	−6.9	−5.0	−4.25
523.16	+7.9	−1.4	−6.3	+0.2	+1.2
523.245	+7.9	−1.4	−6.4	+0.1	+1.00
548.260	+12.1	−1.3	−5.9	+4.9	+5.60
573.16	+15.8	−1.3	−5.5	+9.0	+9.3
573.274	+15.8	−1.3	−5.5	+9.0	+9.80
598.285	+19.1	−1.2	−5.1	+12.8	+13.60
623.295	+22.2	−1.2	−4.8	+16.2	+17.05
673.16	+27.5	−1.1	−4.3	+22.1	+23.6

" Neopentane "

T (°K)	B_{L-J}	B_{anis}	$B_{O-ind\mu}$	B_{O-O}	B_{calc}	B_{obs}[b)]
323.16	−314.5	−0.5	−18.7	−400.3	−734.0	−734
333.16	−294.0	−0.5	−18.1	−375.2	−687.8	−686
348.16	−265.8	−0.4	−17.2	−342.7	−626.1	−626
363.16	−240.2	−0.4	−16.4	−314.9	−571.9	−566
373.16	−224.5	−0.4	−15.9	−299.6	−540.4	−536
383.16	−209.9	−0.4	−15.4	−284.6	−510.3	−507
398.16	−189.5	−0.3	−14.9	−264.5	−469.2	−472
433.8	−147.4	−0.3	−13.5	−225.1	−386.3	−384
448.16	−132.6	−0.3	−13.1	−211.6	−357.6	−356
473.16	−109.2	−0.2	−12.4	−190.2	−312.0	−313
498.16	−88.5	−0.2	−11.7	−173.7	−274.1	−275
523.16	−70.2	−0.2	−11.3	−159.6	−241.3	−244
548.16	−53.7	−0.2	−10.7	−146.9	−211.5	−216

a) M. Douslin, M. Harrison, M. Moore and M. McCullough, *J. Chem. Phys.*, **35**, 1357 (1961).

b) S. D. Hamann and J. A. Lawbert, *Aust. J. Chem.*, **7**, 1 (1954); S. D. Hamann, J. A. Lambert and R. B. Thomas, *ibid.*, **8**, 149 (1955).

estimated from Eqs. (4) and (5). The values of Lennard-Jones (Table 6, a)) were obtained from the analysis of viscosity data in which the effect of octupole mement could be neglected. Average values of the octupole moment for CF_4 and $C(CH_3)_4$ estimated in this way using the observed values of second virial coefficients ***B*** are listed in Table 6, together with the other parameters used in calculations. The second virial coefficients calculated from the average octupole moment in Eq. (4) and the observed second virial coefficients are given in Table 7 for comparison.