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PRESSURE-VOLUME-TEMPERATURE RELATIONSHIPS OF GASES VIRIAL COEFFICIENTS

J. M. H. Levelt Sengers, Max Klein, and John S. Gallagher

Heat Division
National Bureau of Standards
Washington, D. C.

March 1971

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NOTICES

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FOREWORD

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This technical report has been reviewed and is approved.

Michael G. Buja	Harry L. Maynard
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Research and Development Division	Director of Technology
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ABSTRACT

Tables of second virial coefficients as functions of temperature are presented for 14 gases. These gases are mainly noble gases and constituents of air. In most cases, these are based on a reexamination of the original P-V-T data. Where necessary and possible, these data have been refitted and improved experimental virials determined. In the case of eight of these gases, it has been possible to fit the experimental second virials to those predicted by the (m, 6) potential function and potential parameters determined. In almost all cases, an optimum fit was obtained for $m = 18$. The optimum potential function was used for extrapolating the tables somewhat beyond the experimental range, and for obtaining temperature derivatives of B. In the case of the other six substances virial coefficients predicted by the (m, 6) functions were used as a smoothing aid. Experimental third virial coefficients are presented at the experimental temperatures. A table of Boyle and Joule-Thomson inversion temperatures is also presented.

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SECTION I
INTRODUCTION

DEFINITION

Virial coefficients are the coefficients in the expansion of the compressibility factor PV of a gas in powers of the density 1/V:

$$PV = RT\ [1 + B_V/V + C_V/V^2 + \ldots] \tag{1}$$

or in powers of the pressure P:

$$PV = RT\ [1 + B_P P + C_P P^2 + \ldots] \tag{2}$$

The density expansion is the more fundamental of the two. It can be proven that such an expansion exists for gases at moderate densities, and its consecutive coefficients can be related to interactions between pairs, triplets ... etc. of molecules.[1] The pressure expansion is often more practical, the pressure being more readily measured than the volume, but it usually converges slower and its coefficients are not as simply related to molecular interaction. In what follows, the emphasis will be on the expansion(1).

UNITS

The units of the virials depend on the units of volume (1) or pressure (2) chosen. We will express the volume in cm³/mol and give the virials in the corresponding units. However, a practical unit of volume frequently used is the Amagat unit; the volume in Amagat units is the ratio of the actual volume of a gas over the normal volume, i.e., that which it would occupy at 0°C and 1 atm (1.013250 bar). The normal volume for a mol of a real gas differs slightly from the normal volume V_o = 22,413.6 cm³/mol of a perfect gas, due to deviations from ideality at 0°C and 1 atm. The virial expansion used in conjunction with Amagat units of volume is:

$$PV_A = A_A + B_A/V_A + C_A/V_A^2 + \ldots \tag{3}$$

In Table 1, the virials B_P, C_P; A_A, B_A, C_A; are expressed in terms of B_V, C_V.

THEORETICAL INTEREST

Of great interest is the fundamental relationship of B_V, C_V, ... to the molecular interaction. If the molecular field is represented by a function $\phi(\vec{r})$ where $\vec{r}$ specifies the relative coordinates of two molecules, then

$$B_V\ (T) = \frac{N}{2} \int_0^\infty (1 - e^{-\phi(r)/kT})\ d\vec{r} \tag{4}$$

The virial B_V (T) is uniquely determined through (4) if the molecular interaction $\phi(r)$ is known but the reverse is not true. Higher virials can be likewise related to interactions between triplets, etc., of interacting molecules. These expressions for the higher virials are less useful in practice, not only because the higher virials are poorly known experimentally, but also because the influence of potential function non-additivity[1] on these virials is poorly known theoretically. We have used the relationship (4) between second virial and potential function for smoothing the experimental B(T) values, for obtaining derivatives dB/dT, d^2B/dT^2, and where reasonable, for extrapolating the B(T) tables beyond the temperature range where experimental data are available.

PRACTICAL IMPORTANCE

The virials B_V and C_V represent the initial deviations of the equation of state from ideality as a gas is compressed, (1,2). Functions of these virials serve to estimate the initial density dependence of thermodynamic properties. Thus, the internal energy $U_i = U(V, T) - U(\infty, T)$ is given by

$$U_i = -RT \frac{T}{V} \frac{dB_V}{dT} + \frac{T}{2V^2} \frac{dC_V}{dT} + \ldots ,$$

Similar expressions are valid for other thermodynamic functions.[2]

SECTION II
METHODS USED

DETERMINATION; ERRORS

Virial coefficients, in the majority of cases, are not directly measured but are obtained by analysis of PVT data of gases. The most common practice is a least-squares fit of the PV values along isotherms with either density or pressure as an independent variable. Using this procedure, the precision of the virials can then be obtained from linear least-squares estimates of their standard deviations. For a single experimental set in the very best cases, it may be better than .1 cm^3/mol for B and 50 cm^6/mol for C. However, virial data from different experiments usually differ by much more than their combined precision due to the presence of systematic errors. The main sources of systematic errors are:

1. Experimental: (a) errors in the value of RT because of temperature errors or the use of scales other than the thermodynamic scale; (b) systematic errors in the volume because of calibration problems and (c) difficulties with extrapolation to zero density, especially with data obtained by the Burnett method.[3]

2. Cut-off Problems: A finite polynomial has to be used rather than the theoretically correct infinite series (1,2) but errors arise if the powers omitted would have contributed in the density range studied.

To minimize systematic errors, if there was evidence that there were any, we have refitted the experimental data when available. The data refitted are indicated by asterisks in the literature reference for the tables. Wherever feasible, we reduced temperatures to the thermodynamic scale, using the known relation between this scale and the IPTS.[4] If a laboratory maintains its own gas scale, this scale was used. In a few cases, notably He at low temperatures, where one of the purposes of the experiment was gas thermometry, we had to leave the intercept free. Regarding the cut-off criterion[5], we chose the maximum density range in which the $(k + 1)^{th}$ virial is necessary. In cases where it could not be obtained from the data, we used the theoretical value as calculated for the Lennard-Jones 6-12 potential. This procedure was justified since only order of magnitude estimates were needed.

After second and third virials had been obtained from each set of experimental data for a given substance, and after obviously wrong results had been eliminated, a smoothing or averaging procedure was established. Use was made of the fundamental relation (4) between the second virial coefficient and the intermolecular potential.

POTENTIAL FUNCTIONS—DETERMINATION, USE

Equation (4) applies to substances for which quantum effects are negligible. For such substances, (4) is exact. Quantum effects become important for only the lightest gases[6], e.g., helium, hydrogen, etc. These latter are generally referred to as quantum gases. For such gases, (4) can only represent a first approximation whose quality goes down with decreasing molecular weight. In either case, i.e., whether (4) is exact or an approximation, the use of (4) requires a knowledge of the intermolecular potential function, $\phi(r)$. In principle such functions can be obtained by direct quantum mechanical calculation. In practice, this procedure is not feasible even for the simplest system. This has required, in effect, the partial reversal of the process. Thus, instead of using (4) with a known function $\phi(r)$ to predict $B(T)$, one uses (4), in part, to produce information on $\phi(r)$ and, in part, to predict $B(T)$. This is done by assuming a form for $\phi(r)$, (often referred to as a potential model), based on whatever fundamental knowledge there is, inserting a number of parameters in this form, (for example ε and σ of (5)), and varying the values of these parameters to obtain the best agreement between the $B(T)$ values calculated from (4) and those determined from the analysis of PVT data described above. The predictive power of (4) remains essentially intact provided the number of experimental points used is far in excess of the number of parameters sought. Frequently used in this way to describe the intermolecular potential of simple nonpolar substances is the Lennard Jones 12-6 potential, a member of the more general class of spherically syymmetric m-6 potentials:

$$\phi(r) = \frac{m\varepsilon}{m-6} \left(\frac{m}{6}\right)^{6/(m-6)} \left[\left(\frac{\sigma}{r}\right)^{m} \quad \left(\frac{\sigma}{r}\right)^{6} \right] \tag{5}$$

where ε and σ are parameters to be determined for each substance. This expression, with proper choice of m, adequately describes the second virial coefficient of simple nonpolar substances.

It should be noted that once a "best" set of parameters is decided upon, one has a potential function which can serve as a representation for the "actual" potential function appropriate to the gas of interest. The use of such potential functions need not be restricted to (4). They can also be used in various statistical mechanical theories for calculating macroscopic thermodynamic quantities from molecular properties. In short, these potential functions have their own importance.

Various methods, of which the use of (4) is only one example, by means of which potential parameters are determined from experimental data have recently been subjected to close scrutiny.[7] In that study it was determined that all reasonable three parameter potential models should produce essentially the same set of second virial coefficients. Because of this it was reasonable to fix on one particular model and we chose (5) for that purpose. A second result of the study of methods for determining potential parameters was the discovery of a reduced temperature range, for each property, over which that property cannot be used to distinguish between potential functions. For the second virial coefficient, this range is given approximately by $0.6<T/T_{Boyle}<3.0$. We have included a table (Table 17) of experimental Boyle temperatures to facilitate the conversion of these numbers into experimental temperatures for the various gases studied. The second result mentioned states, in effect, that one should not use (4) with a potential function determined by data entirely contained in the insensitive range to predict B(T) outside that range; nor should one use the resulting potential function in other theories. On the other hand, potential functions determined with data entirely outside the insensitive range can be used in an extrapolation to predict B(T) values within that range.

CONSTRUCTION OF THE TABLES

Using linear and nonlinear[8] least squares techniques, calculated second virial coefficients based on the function (5) were fitted to the experimental second virial coefficient data for eight substances. Each value of m was taken to define a separate potential with ε and σ in (5) the adjustable parameters for the fit. The value of m was varied until the standard deviation of the fit was a minimum. The "best" m-6 potential was used to generate a table of B, T^2dB/dT and $T^2\ d^2B/dT^2$ values at various temperatures. Furthermore, it was used for extrapolation beyond the range of experimental data. Such extrapolations are indicated in each case by a dashed line across the tables.

Equation (4) and the procedures described above were used for the quantum gases He, H_2 and D_2 as well. In these cases, however, the methods were used only to facilitate smoothing and interpolation of virial data. For H_2O, D_2O and CO_2 a potential of the form (5) was found to be inadequate. These substances were therefore treated as were the quantum gases; that is, the methods outlined were used only for smoothing and interpolation. The tables prepared for these six substances consist only of smoothed experimental B(T) values, with no extrapolations attempted. Tables of T dB/dT and $T^2\ d^2B/dT^2$ are not given nor are potential parameters used in the smoothing process reported since they are without clear meaning. Since the B(T) tables for these six substances are so closely tied to the experimental values, minor departures from smoothness in the tables may be detected.

Third virials, in all cases, were obtained by graphical interpolation of the (refitted) experimental values for C. They are summarized in Table 16.

Table 17 contains values for the Boyle temperature and the inversion temperature. In those cases where the form (5) for the intermolecular potential applies, the potential parameters and the value of m are summarized in Table 18.

We note that the optimum value of m is much closer to 18 than to the popular value of 12.

SECTION III
DISCUSSION

ACCURACY OF TABLES

From a computational point of view, in all cases, the temperature spacing is sufficiently fine to allow for an interpolation to be made using a quadratic formula without the introduction of errors. Furthermore, linear interpolation can be used without introducing an error of more than 0.3 cm^3/mol in B(T) due to the neglect of quadratic terms. It should be noted that where B, TdB/dT, and $T^2\ d^2B/dT^2$ are available, a Taylor series expansion can be used for interpolation.

It is much harder to assess the absolute accuracy of the tables in any general way. Where data from many sources are available for one substance, as in the case for most of the noble gases and for nitrogen, one usually finds discrepancies up to 1.5 cm^3/mol in B and up to 30% in C between data from different laboratories. Discrepancies in B may become much larger at temperatures below critical. The main source of oxygen data (L.A. Weber) is particularly precise, ~ 0.1 cm^3/mol in B, and agrees with the others within combined precision. For hydrogen and deuterium, problems with the temperature scale between 100 and 273K may cause errors in B as large as .5 cm /mol. For H_2O and D O, there is only one source for which the precision ranges from several cm^3/mol at the lower temperatures to .2 cm^3/mol at the higher ones. For CO_2, discrepancies of several cm^3/mol in B exist between data of different sources, and for CH_4, of 0.7 cm^3/mol in B and of 10% in C.

USE OF THE TABLES

The averaged virials presented here can be used for calculations of precise PV products at low pressures. However, in the process of separately averaging and rounding the second and third virials, correlations in their experimental errors have been obliterated; thus, they cannot be used to represent the PVT data from which they were derived within experimental precision over the entire density range. If precise PVT values are needed at higher densities it is usually preferable to interpolate in the original data.

The tables of virials and their temperature derivatives can be used to calculate the initial density dependence of other thermodynamic properties.[2]

DISCUSSION OF THE DEVIATION PLOTS

Figures 1 through 16 contain plots of the deviations of "experimental" second virial coefficients from the tabulated values of Tables 2-15. In some cases, error bars are presented to indicate the estimated precision of the reported values. The figures also contain dashed horizontal lines to indicate the limits $\pm\sigma$ and $\pm 2\sigma$, the latter containing half as many dashed per unit length as the former.

In some instances, experimental values which differed from the least square representation by more than ±3σ were deleted. In one or two instances such points were not deleted either because they were end points or, because there existed points in the same temperature range which differed from the least square fit by a slightly smaller (<3σ) amount of opposite sign. In the latter case the omission of these points would prejudice the fit in favor of other points of equal weight. Data from a laboratory which showed a strong systematic trend away from several other sets of data were not included in the fit and so do not appear in the plots.

It should be noted that where a representation derived from an intermolecular potential function was used, that fact is contained in the figure caption. Where, for reasons already discussed, such a representation was not appropriate, the figure caption refers to the use of a smoothed representation of experimental data.

In two instances, namely helium and carbon dioxide, the experimental data cover such a large range that a second plot covering the low temperature range was included in order to present more detail in the range containing most of the data.

In many instances, there is a tendency for the data from several laboratories to be internally consistent and highly precise but to differ from each other by much more than their combined precision. This is particularly dramatic in the case of xenon (Figure 6) and to a lesser extent for helium (Figure 1), neon (Figure 3) and carbon dioxide (Figure 15). This can be taken as an illustration of the difference between the precision of a measurement and its accuracy.

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APPENDIXES

I. ILLUSTRATIONS
II. TABLES

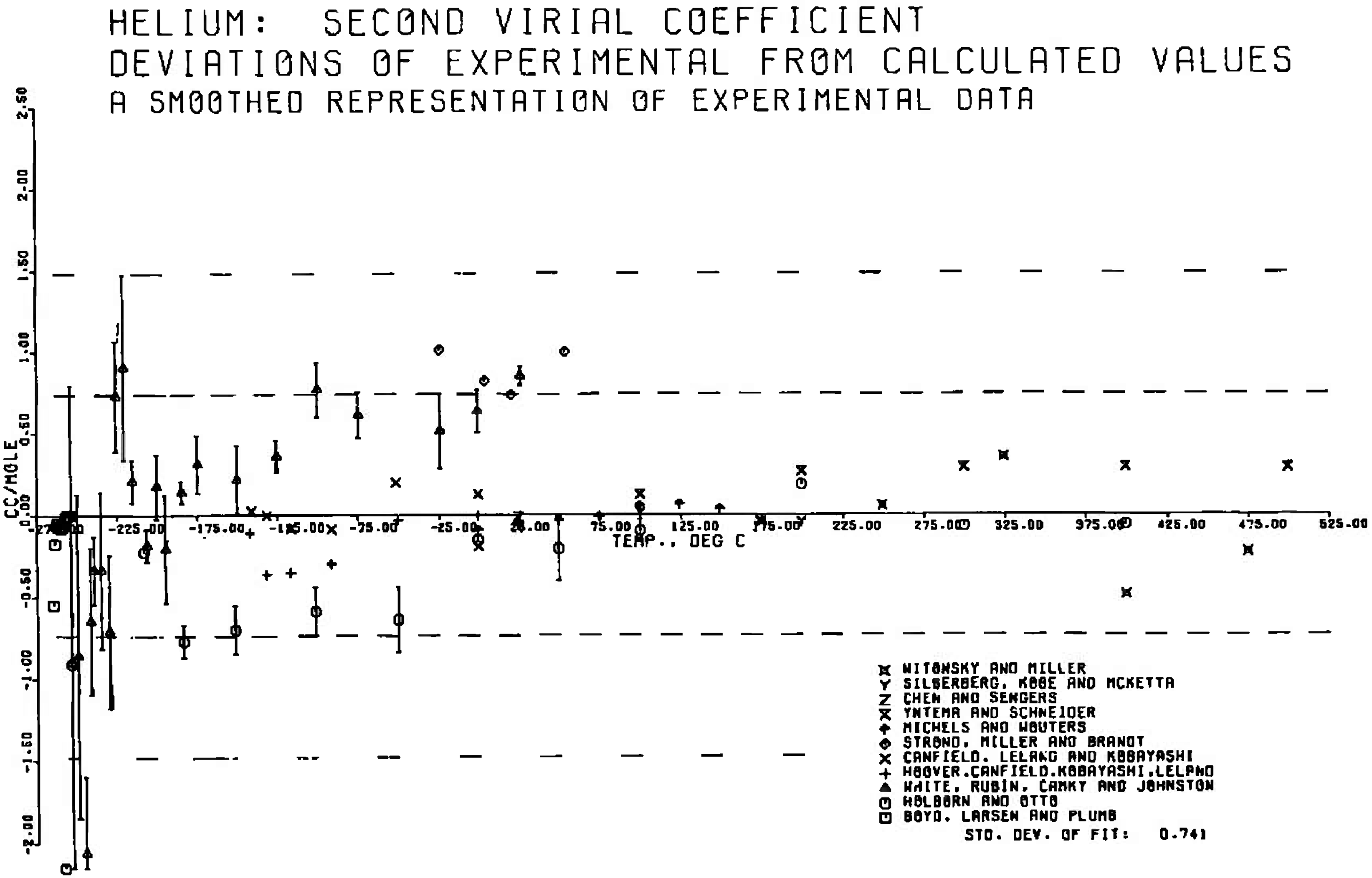

Fig. 1 Deviation Plots for Helium (TL < 525°C)

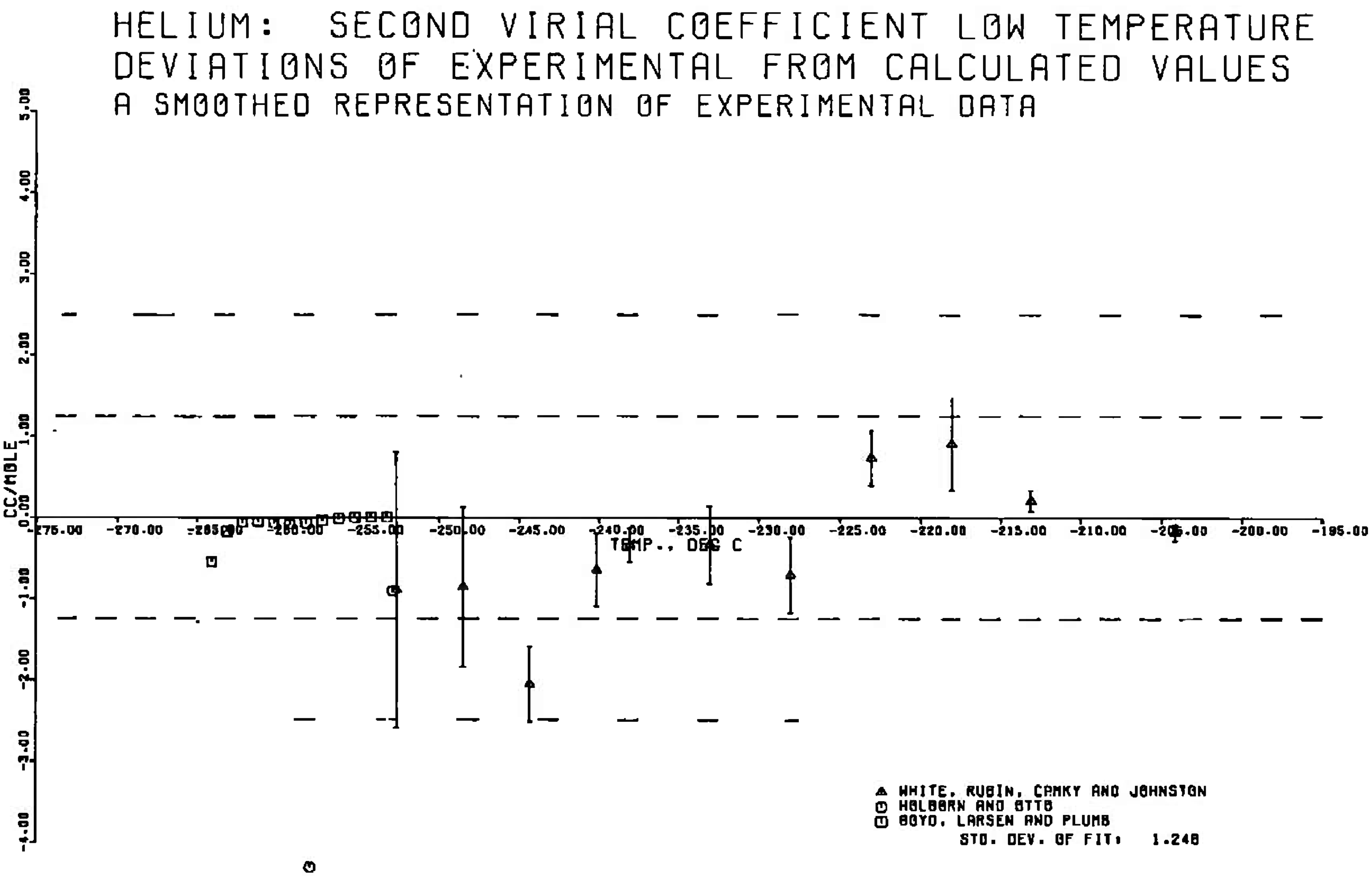

Fig. 2 Deviation Plots for Helium (T < -195°C)

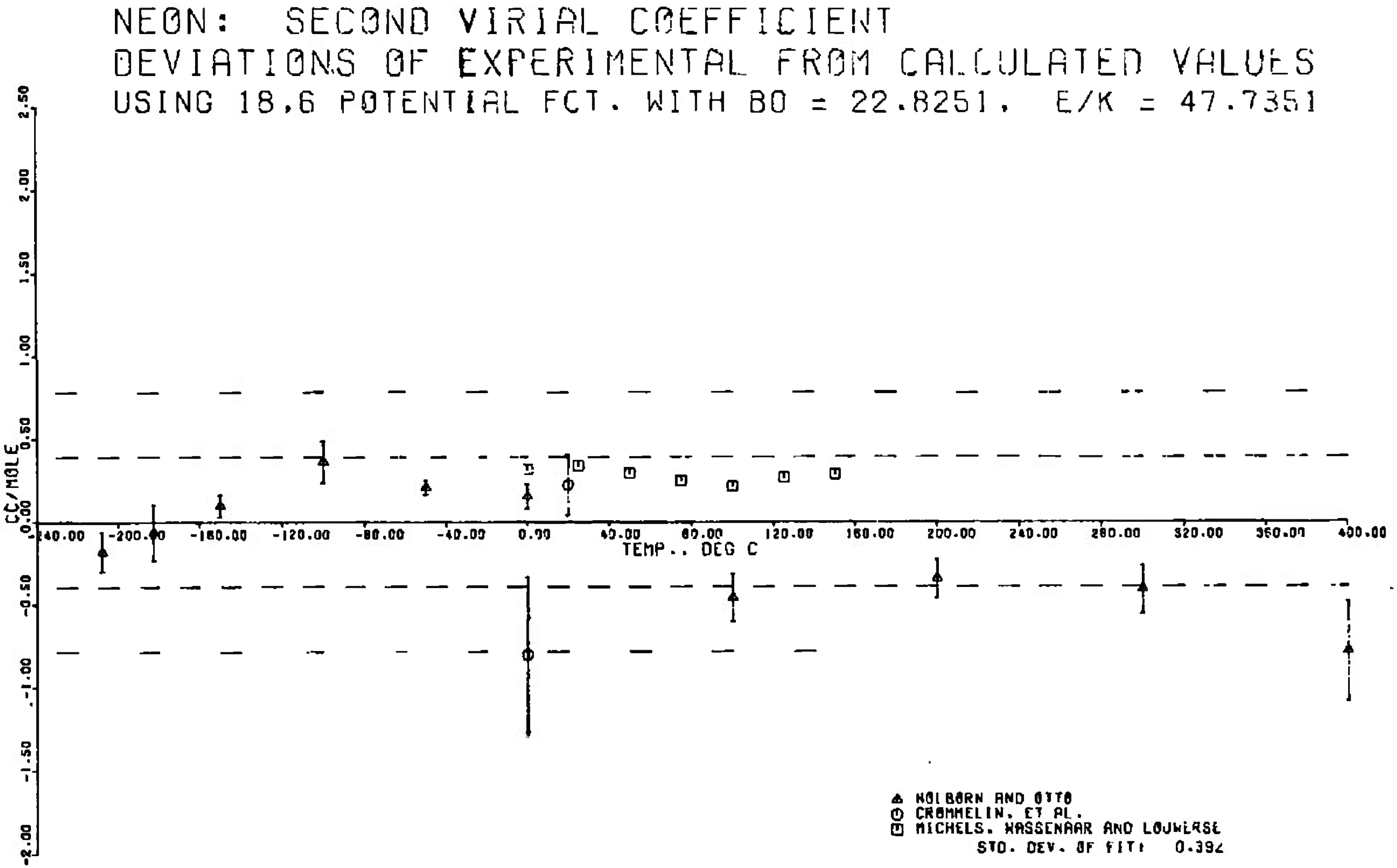

Fig. 3 Deviation Plots for Neon

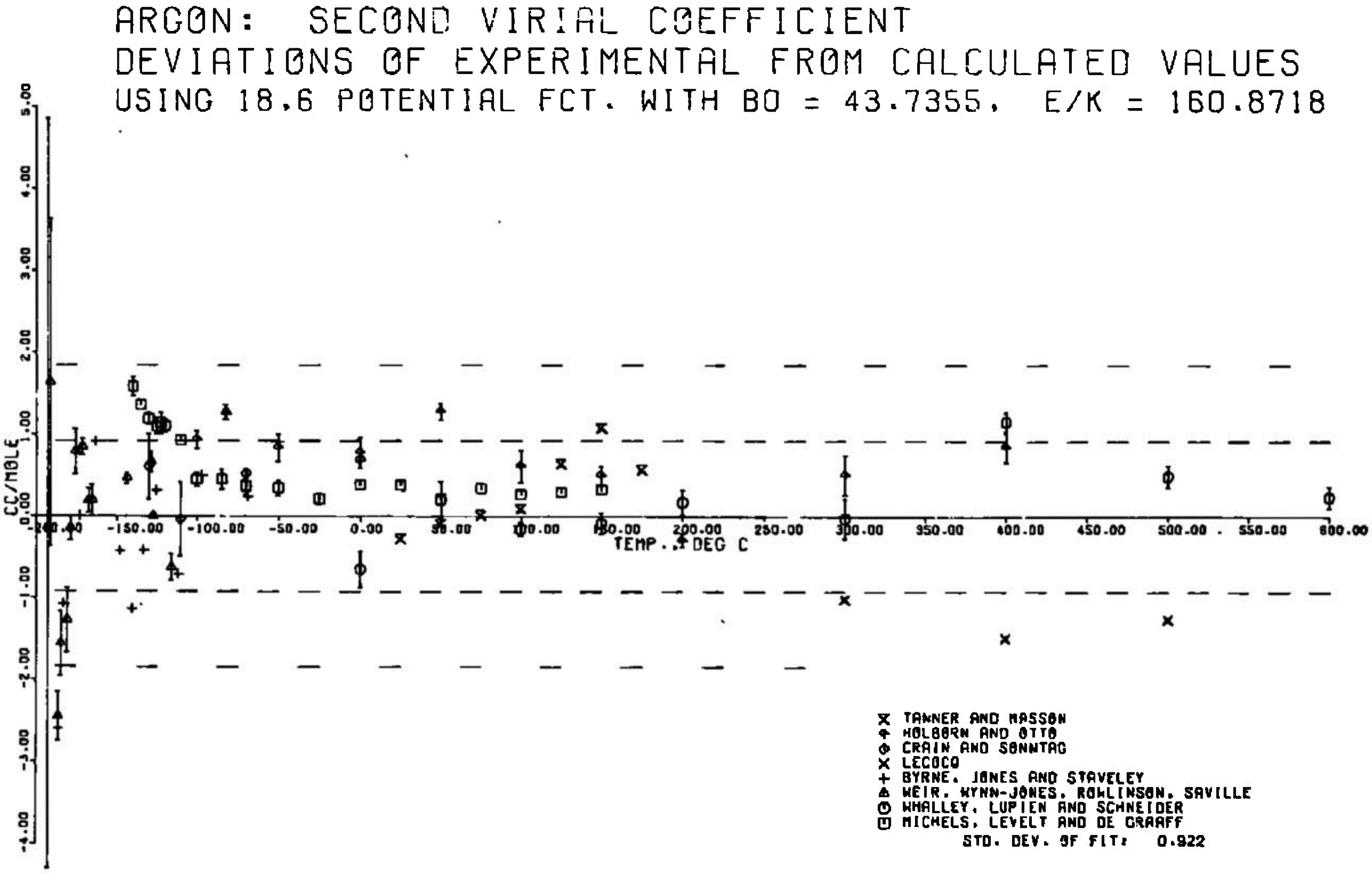

Fig. 4 Deviation Plots for Argon

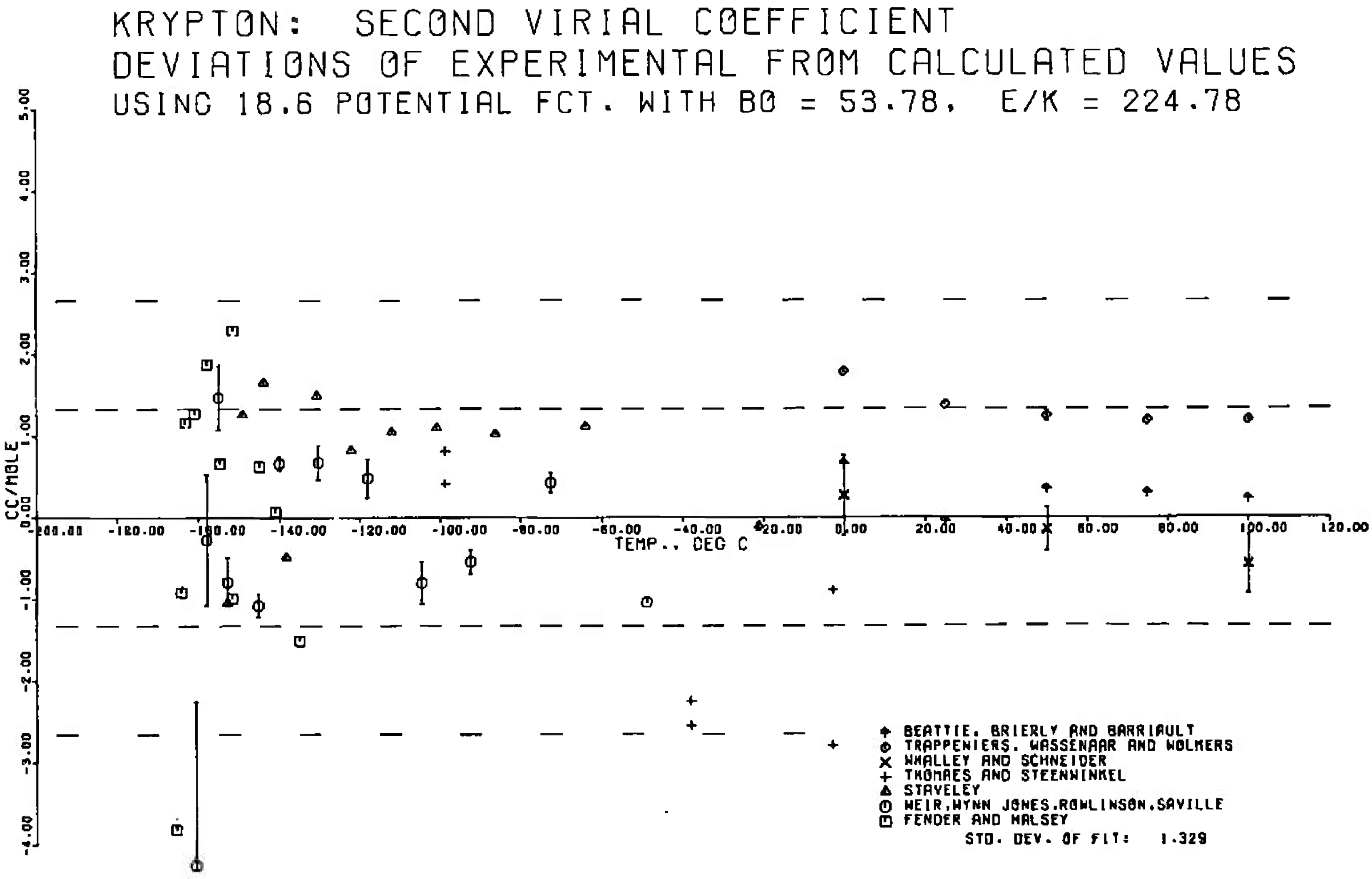

Fig. 5 Deviation Plots for Krypton

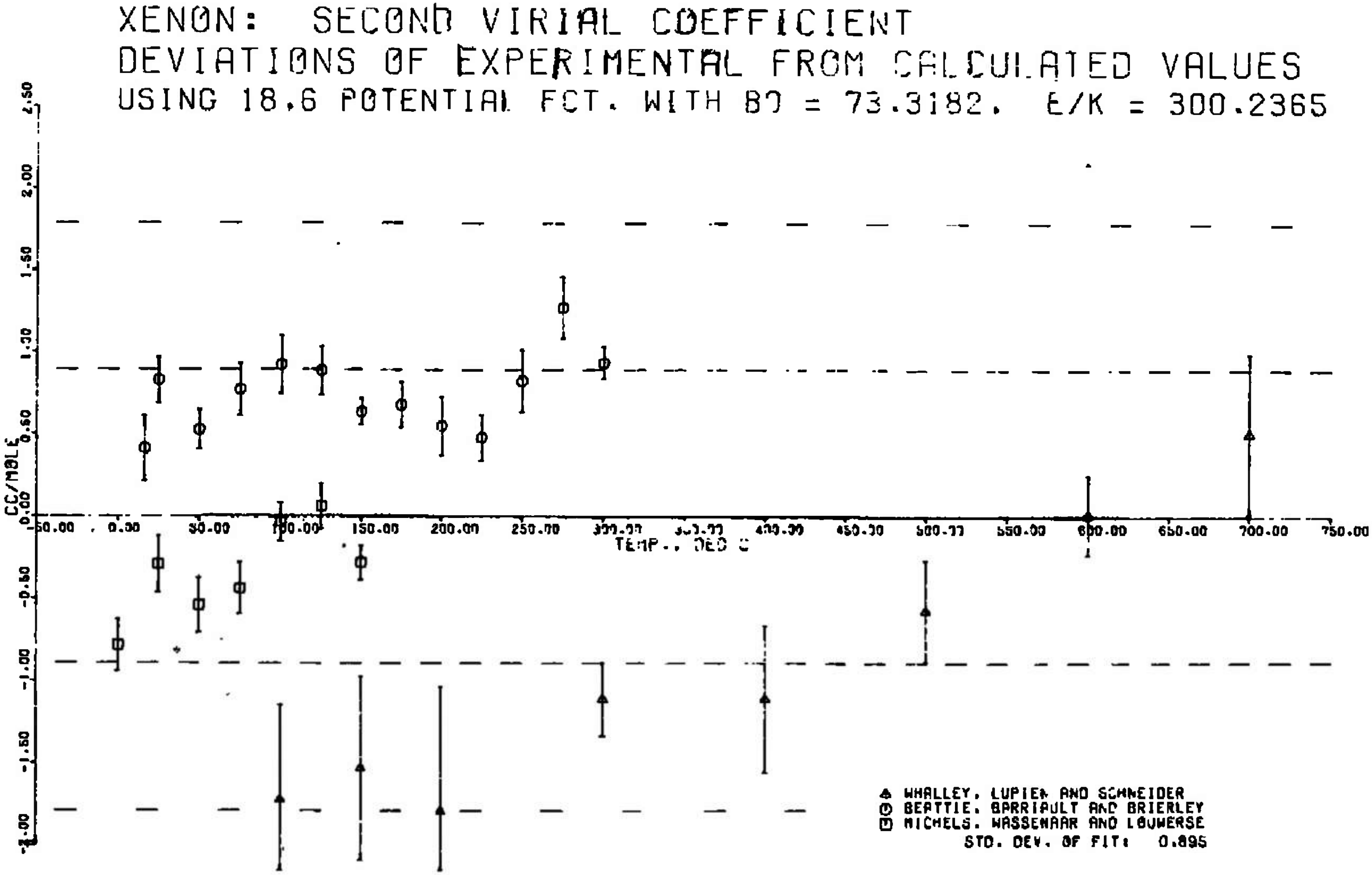

Fig. 6 Deviation Plots for Xenon

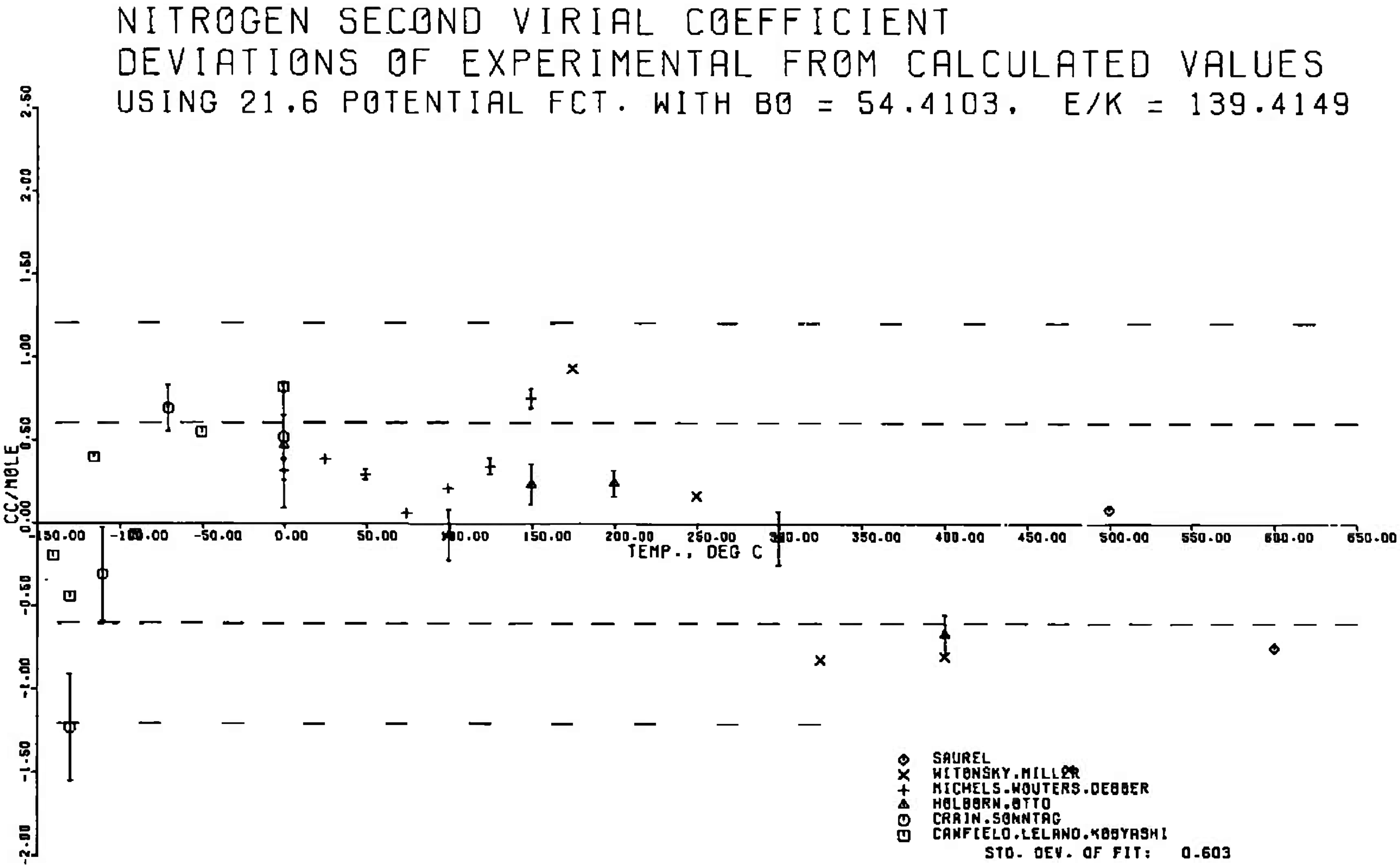

Fig. 7 Deviation Plots for Nitrogen

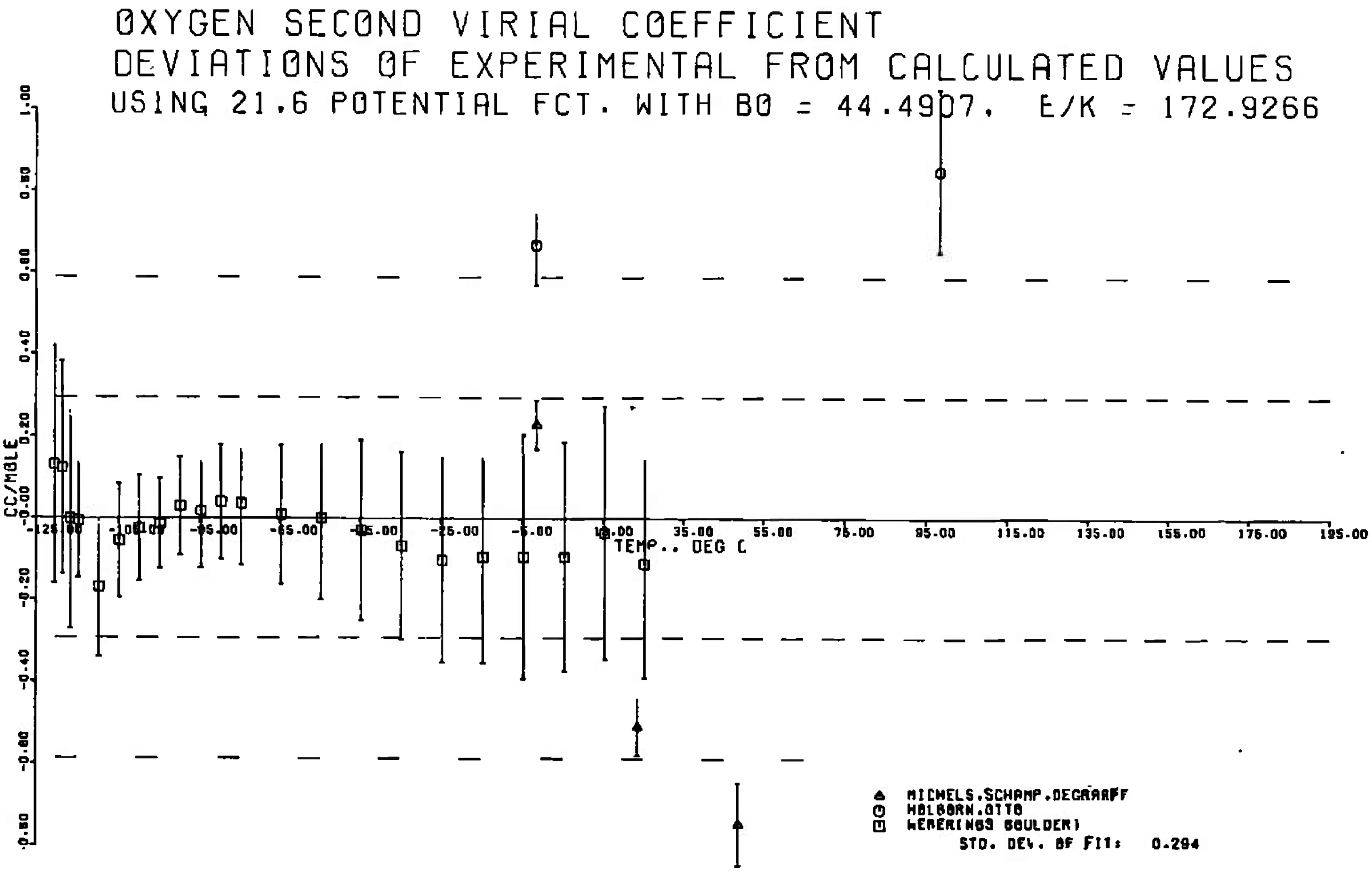

Fig. 8 Deviation Plots for Oxygen

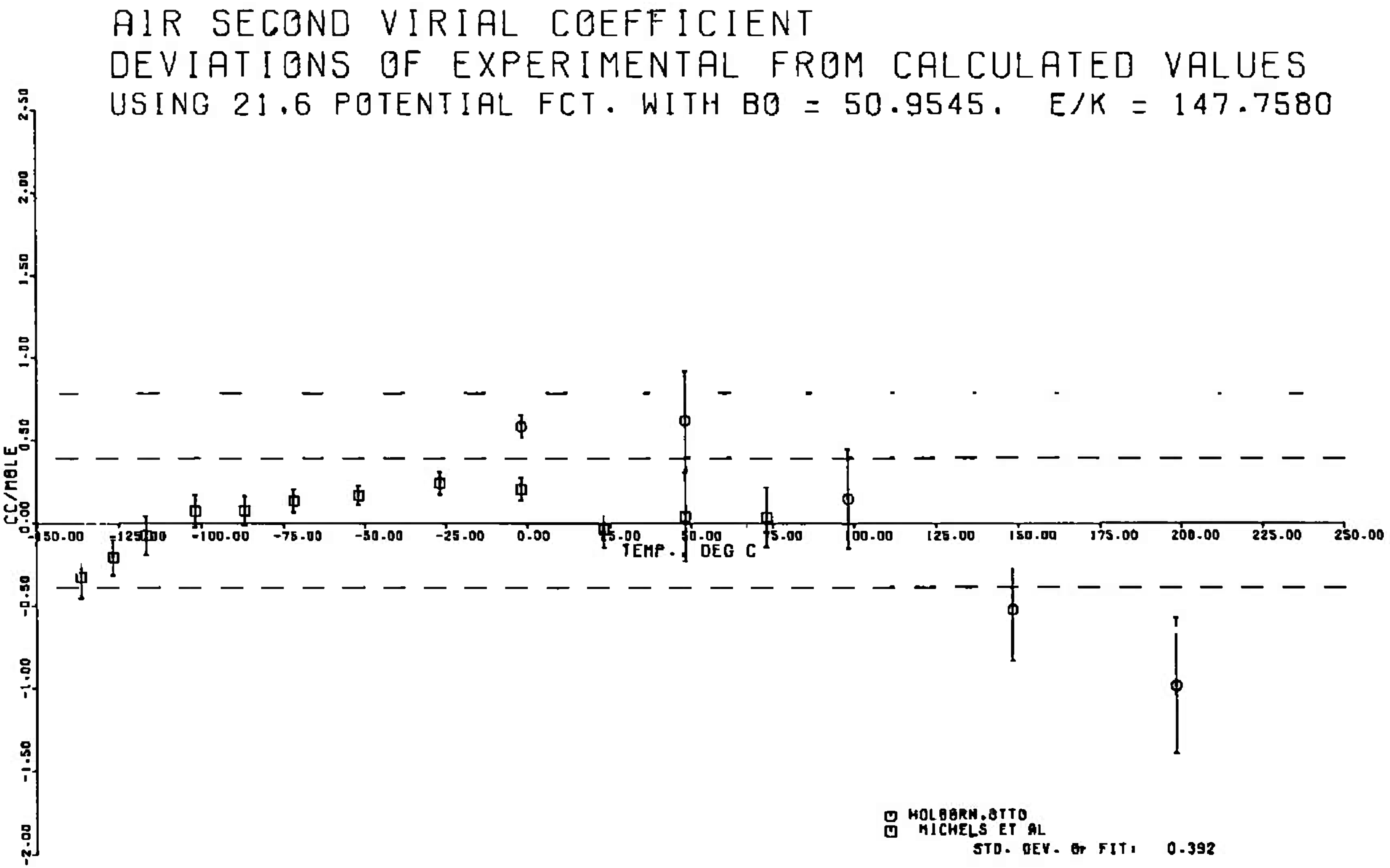

Fig. 9 Deviation Plots for Air

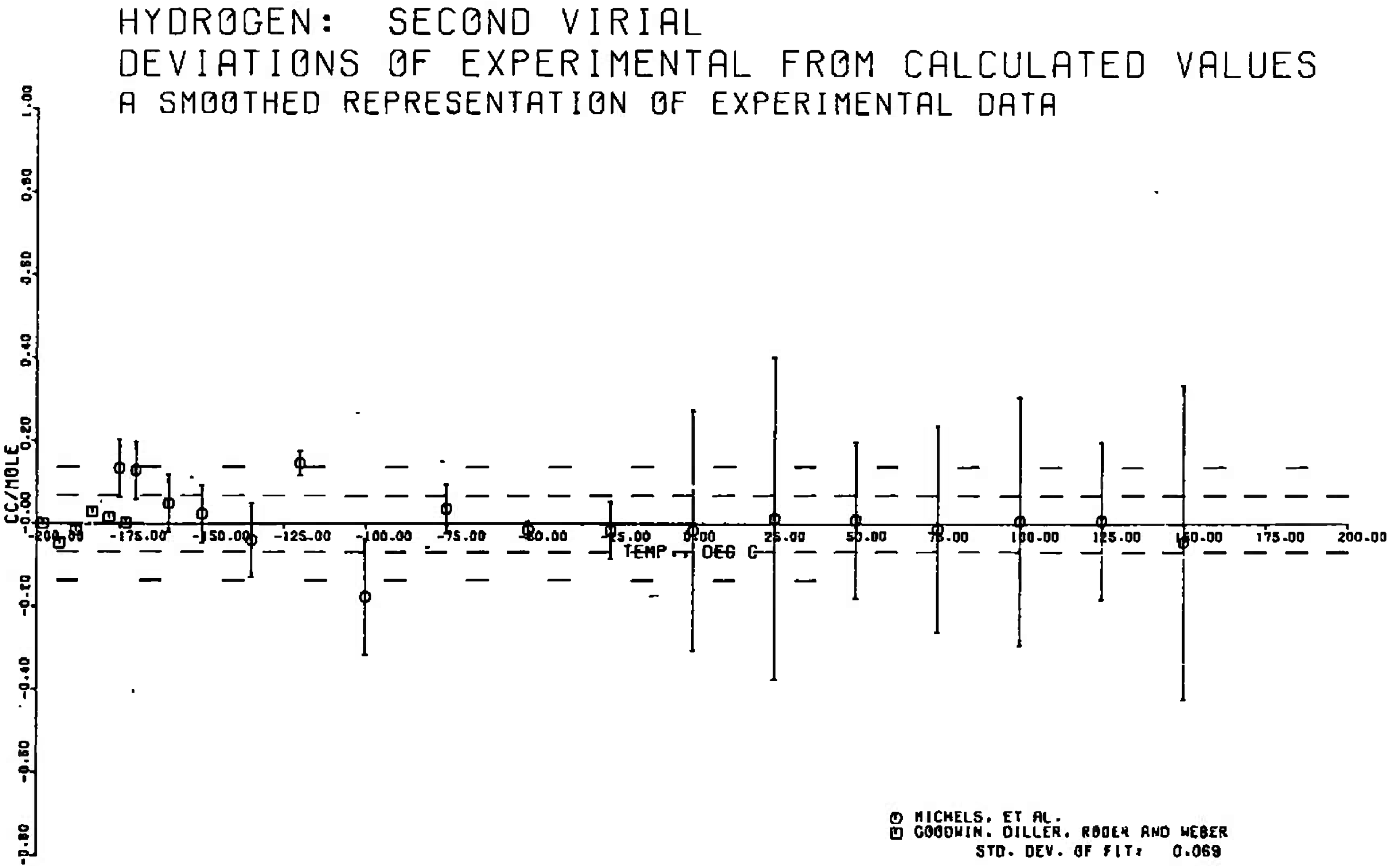

Fig. 10 Deviation Plots for Hydrogen

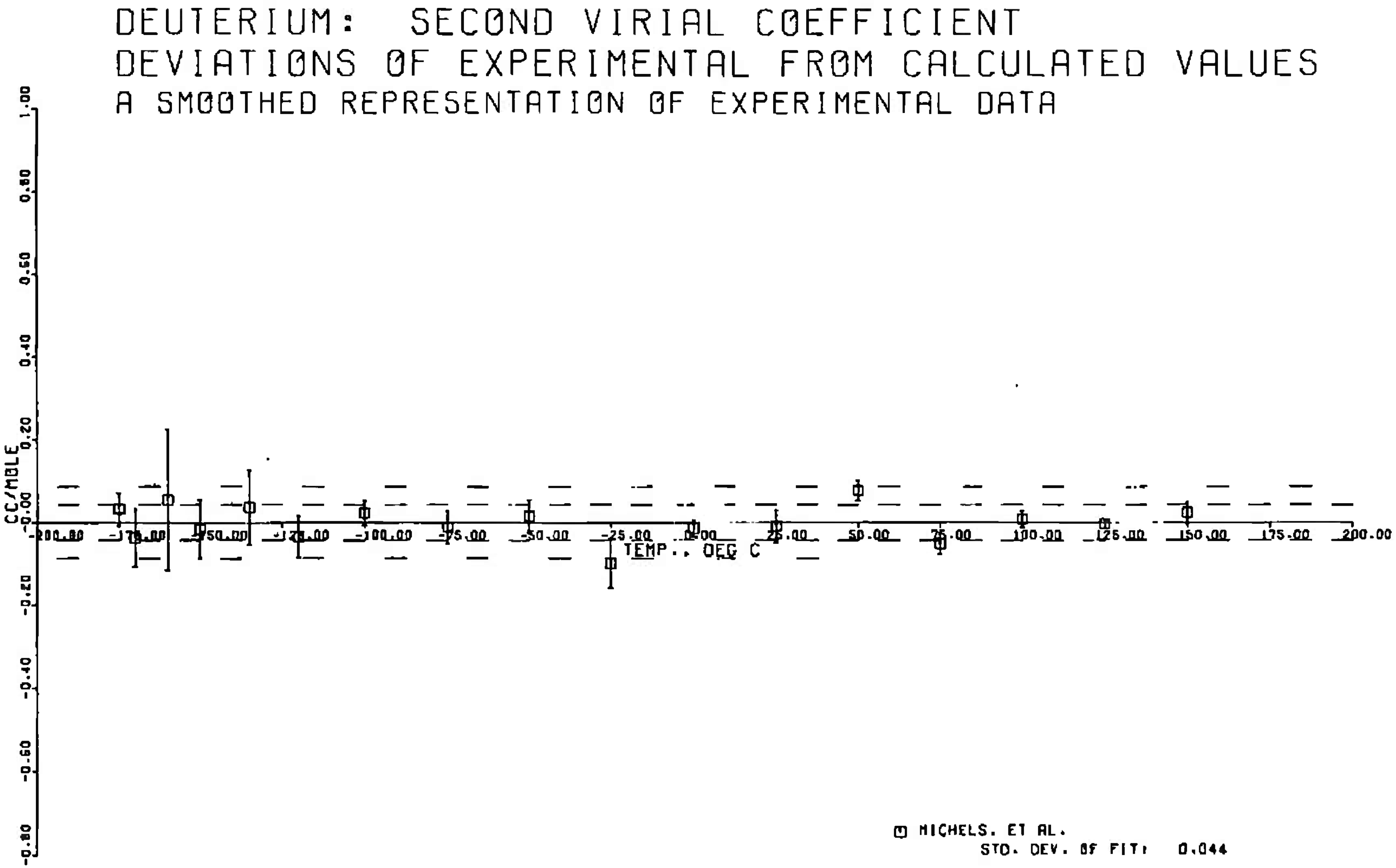

Fig. 11 Deviation Plots for Deuterium

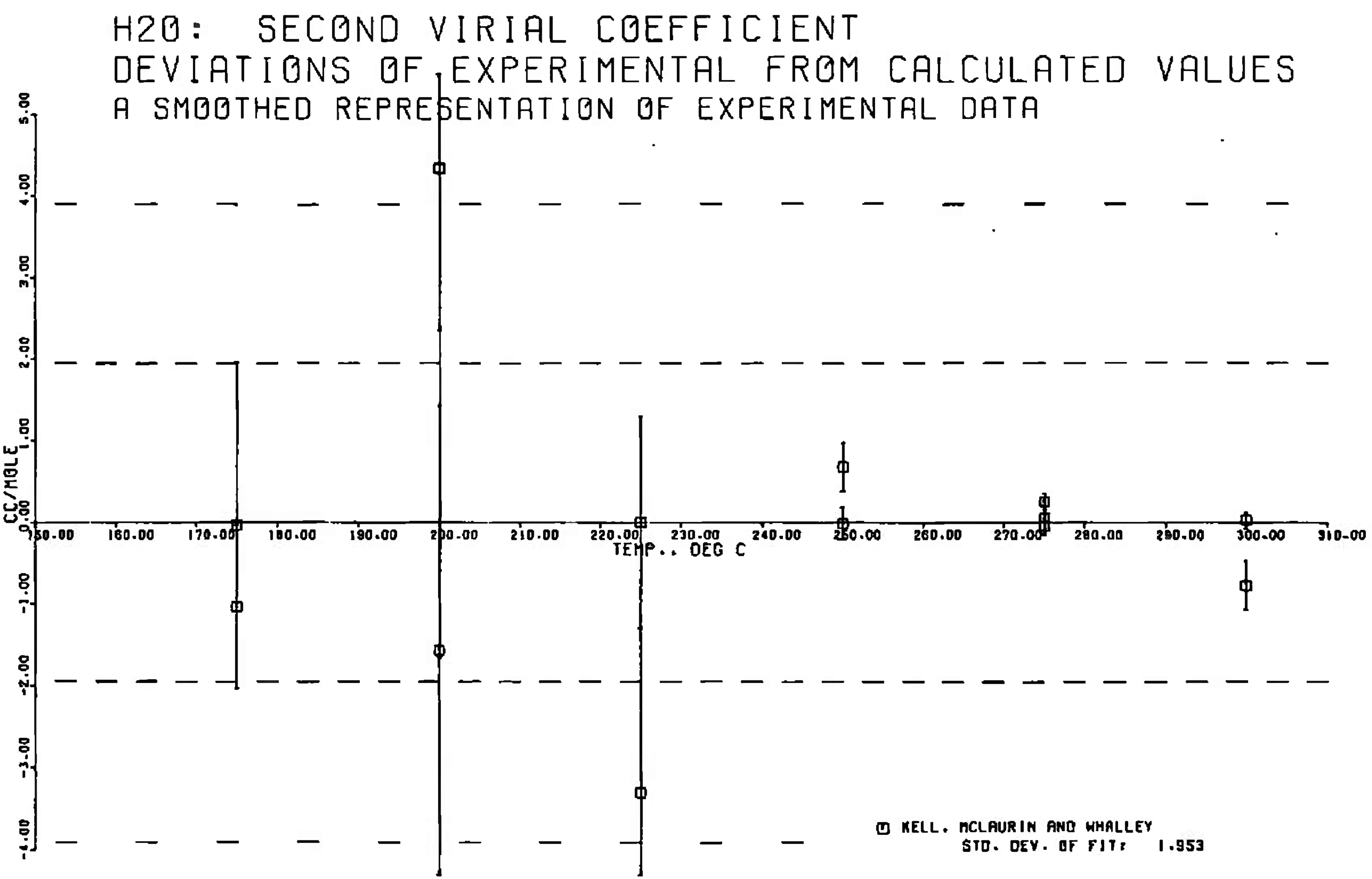

Fig. 12 Deviation Plots for H_2O

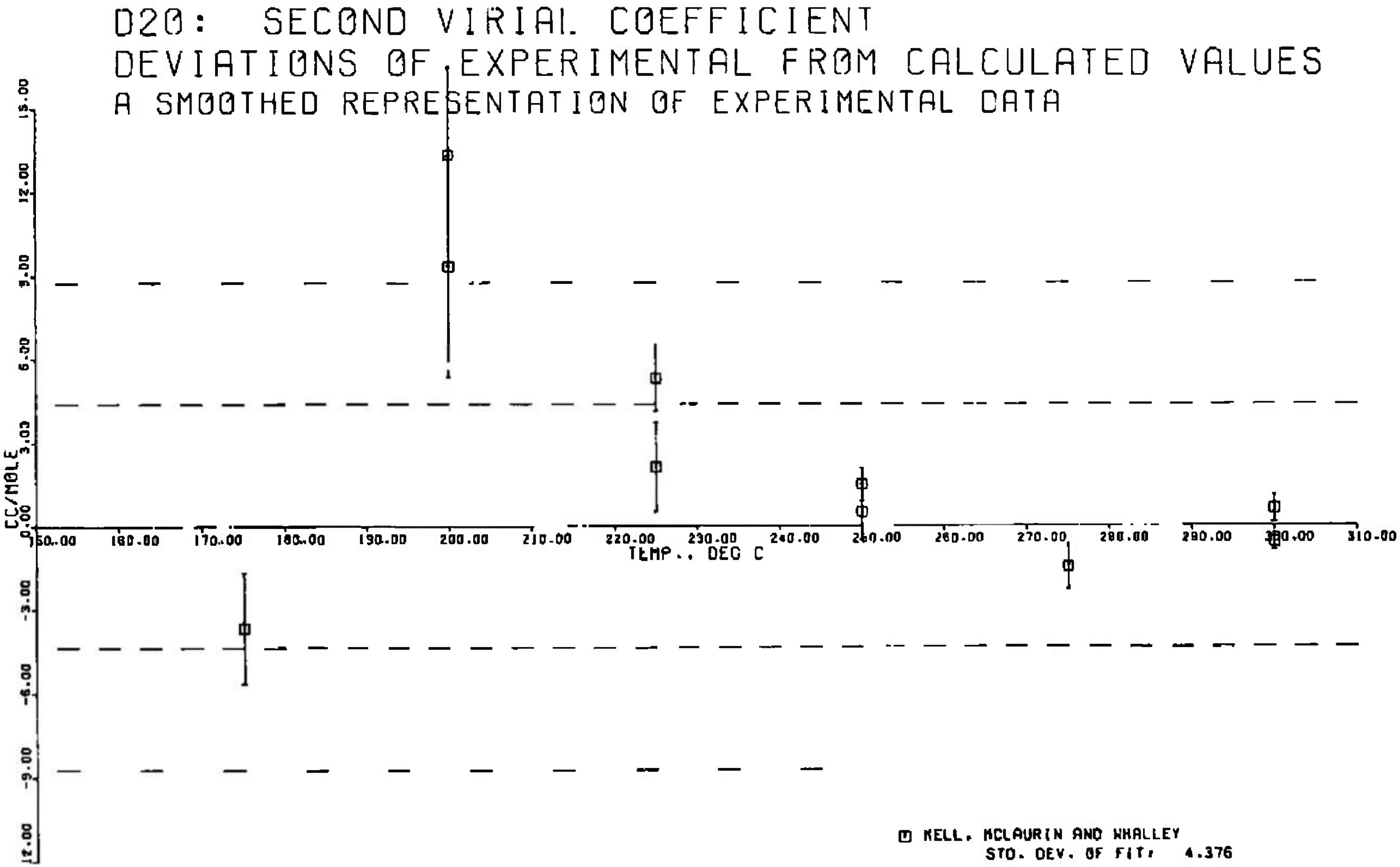

Fig. 13 Deviation Plots for D_2O

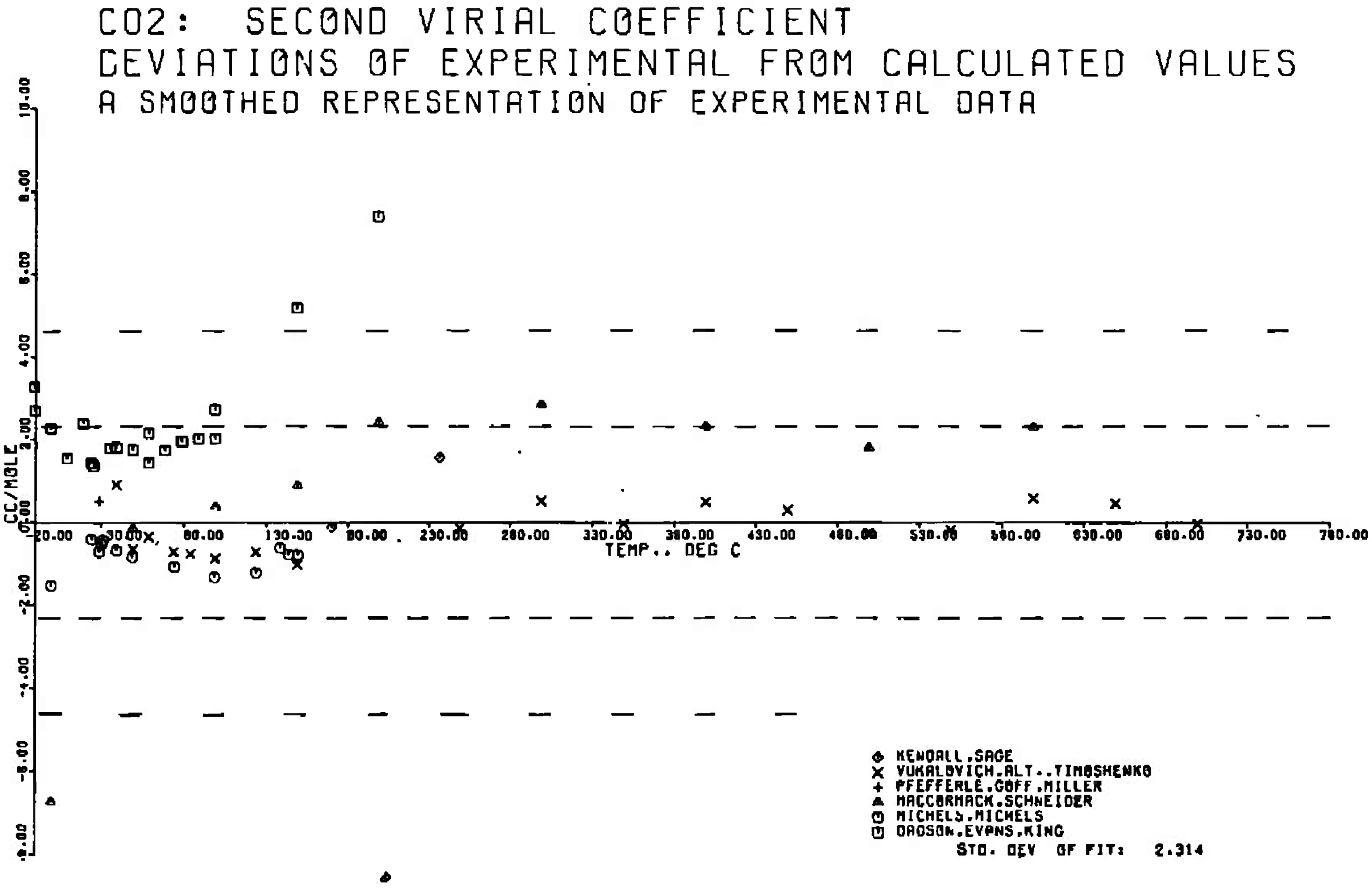

Fig. 14 Deviation Plots for CO_2 (TL < 780°C)

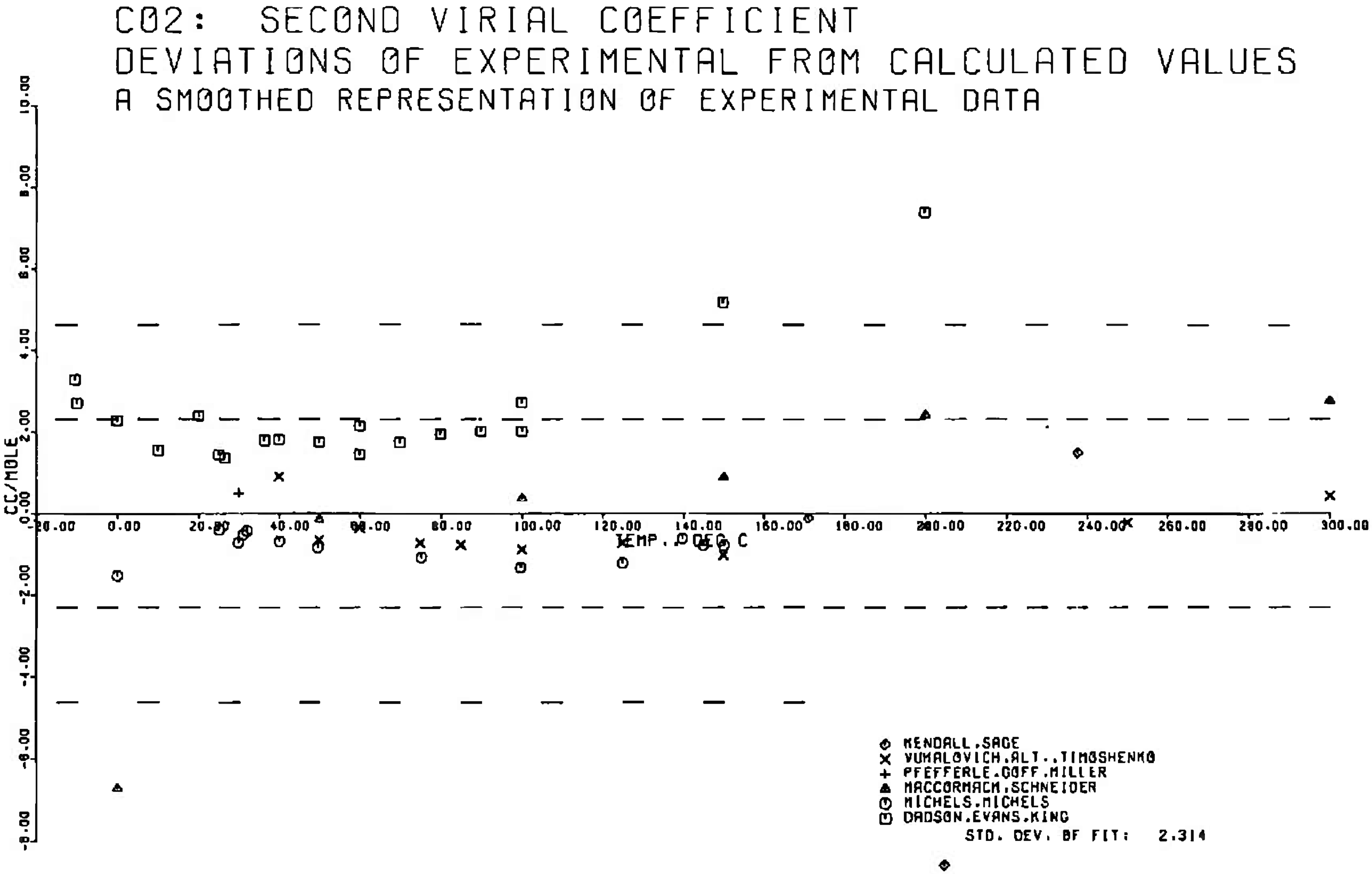

Fig. 15 Deviation Plots for CO_2 (TL < 300°C)

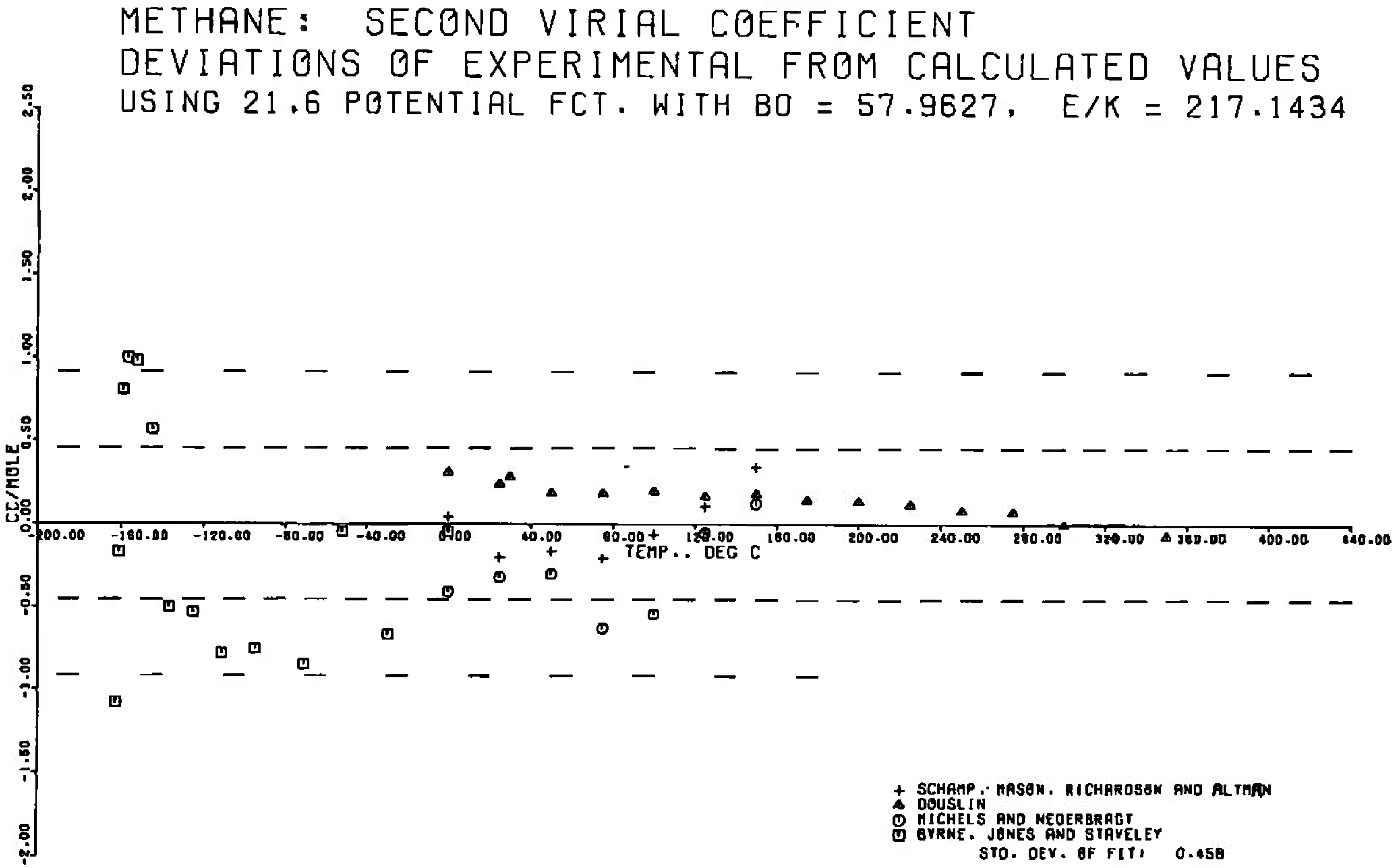

Fig. 16 Deviation Plots for Methane

TABLE 1
RELATIONS BETWEEN VOLUME AND PRESSURE VIRIAL COEFFICIENTS

Gas Constant

$R = 8.3143\ JK^{-1}\ mol^{-1}$

$(= 82.056\ cm^3\ at\ K^{-1}\ mol^{-1})$

Ideal Gas Normal Volume per Mol

$V_o = 22{,}413.6\ cm^3\ mol^{-1}$

(Both on unified scale)

Pressure virials (2)

$B_p = B_V/RT$

$C_p = (C_V - B_V^2)/(RT)^2$

Amagat virials (3)

$V_n = V_o/A_o$

$A_o = 1 - B_A\ (0°C) - C_A(0°C)\ \ldots$

$A_A = A_o T/273.15$

$B_A = B_V\ A_A/V_n$

$C_A = C_V\ A_A/V_n^2\ .$

TABLE 2
SECOND VIRIAL COEFFICIENT OF HELIUM

T K	B cm^3/mol	T K	B cm^3/mol
9.00	-26.0	35.00	5.4
10.00	-21.7	40.00	6.6
11.00	-18.1	45.00	7.5
12.00	-15.2	50.00	8.2
13.00	-12.7	60.00	9.2
14.00	-10.5	80.00	10.6
15.00	-8.7	100.00	11.4
16.00	-7.1	120.00	11.8
17.00	-5.6	160.00	12.3
18.00	-4.3	200.00	12.3
19.00	-3.2	273.15	12.0
20.00	-2.2	373.15	11.3
22.00	-.5	400.00	11.1
22.64	0.0	600.00	10.4
24.00	.9	800.00	9.8
26.00	2.0	1000.00	9.3
28.00	3.0	1200.00	8.8
30.00	3.8	1400.00	8.4

TABLE 3
SECOND VIRIAL COEFFICIENT OF NEON AND ITS TEMPERATURE DERIVATIVES

T K	B cm^3/mol	TdB/dT cm^3/mol	T^2d^2B/dT^2 cm^3/mol
80.00	-11.8	37.	-87.
90.00	-7.8	31.	-73.
100.00	-4.8	27.	-63.
110.00	-2.3	24.	-55.
120.00	-.4	21.	-49.
122.11	0.4	21.	-48.
130.00	1.2	19.	-44.
140.00	2.6	18.	-40.
160.00	4.8	15.	-34.
200.00	7.6	11.	-26.
240.00	9.4	9.	-20.
273.15	10.4	7.	-17.
280.00	10.6	7.	-17.
320.00	11.5	6.	-14.
360.00	12.1	5.	-12.
373.15	12.3	5.	-12.
400.00	12.6	4.	-11.
500.00	13.3	3.	-8.
600.00	13.8	2.	-6.
700.00	14.0	1.	-5.
800.00	14.2	1.	-4.
900.00	14.3	1.	-3.
1000.00	14.3	0.	-3.

TABLE 4
SECOND VIRIAL COEFFICIENT OF ARGON AND ITS TEMPERATURE DERIVATIVES

T K	B cm^3/mol	TdB/dT cm^3/mol	T^2d^2B/dT^2 cm^3/mol
80.00	-288.0	577.	-1954.
82.00	-274.2	544.	-1820.
84.00	-261.4	514.	-1700.
86.00	-249.7	488.	-1592.
88.00	-238.7	463.	-1495.
90.00	-228.6	441.	-1408.
92.00	-219.1	420.	-1328.
94.00	-210.3	401	-1256
96.00	-202.0	384.	-1190.
98.00	-194.3	367.	-1129.
100.00	-187.0	352.	-1074
102.00	-180.2	338.	-1023.
104.00	-173.8	325.	-976.
106.00	-167.7	313.	-932.
108.00	-161.9	302.	-892.
110.00	-156.5	292.	-855.
112.00	-151.3	282.	-820.
114.00	-146.4	272.	-788.
116.00	-141.7	264.	-757.
118.00	-137.3	255.	-729.
120.00	-133.1	247.	-702.
124.00	-125.2	233.	-654.
128.00	-118.0	220.	-612.
132.00	-111.4	209.	-573.
136.00	-105.4	198.	-539.
140.00	-99.8	188.	-509.
144.00	-94.6	180.	-481.
148.00	-89.8	172	-456.
152.00	-85.3	164.	-433.
156.00	-81.1	157.	-413.
160.00	-77.2	151.	-394.
164.00	-73.5	145.	-376.
168.00	-70.1	140.	-360.
172.00	-66.9	135.	-345.
176.00	-63.8	130.	-331.
180.00	-60.9	126.	-318.
190.00	-54.4	116.	-290.
200.00	-48.7	107.	-266.
210.00	-43.7	100.	-245.
220.00	-39.2	93.	-228.
230.00	-35.2	88.	-212.
240.00	-31.5	83.	-198.
250.00	-28.2	78.	-186.
260.00	-25.3	74.	-176.
273.15	-21.7	69.	-163.
280.00	-20.1	67.	-157.
300.00	-15.7	61.	-142.
320.00	-11.9	56.	-130.
340.00	-8.7	51.	-119.
360.00	-5.8	48.	-110.
373.15	-4.2	46.	-105.
380.00	-3.4	44.	-102.
400.00	-1.1	42.	-96.
411.52	0.0	40.	-92.
450.00	3.4	36.	-82.
500.00	6.9	31.	-71.
550.00	9.7	28.	-63.
600.00	11.9	25.	-57.
700.00	15.4	20.	-47.
800.00	17.8	17.	-40.
900.00	19.7	14.	-34.
1000.00	21.1	12.	-30.
1100.00	22.2	11.	-27.
1300.00	23.8	8.	-21.
1500.00	24.8	7.	-18.

TABLE 5
SECOND VIRIAL COEFFICIENT OF KRYPTON AND ITS TEMPERATURE DERIVATIVES

T K	B cm^3/mol	TdB/dT cm^3/mol	T^2d^2B/dT^2 cm^3/mol
106.00	-394.3	807.	-2813.
108.00	-379.6	771.	-2659.
110.00	-365.8	737.	-2518.
112.00	-352.8	706.	-2389.
114.00	-340.5	677.	-2270.
116.00	-329.0	650.	-2160.
118.00	-318.1	625.	-2059.
120.00	-307.8	601.	-1965.
122.00	-298.0	579.	-1878.
124.00	-288.8	559.	-1797.
126.00	-280.0	539.	-1722.
128.00	-271.6	521.	-1651.
130.00	-263.7	504.	-1586.
132.00	-256.1	488.	-1524.
134.00	-248.9	473.	-1467.
136.00	-242.0	458.	-1413.
138.00	-235.4	444.	-1362.
140.00	-229.1	432.	-1314.
144.00	-217.3	408.	-1226.
148.00	-206.4	386.	-1148.
152.00	-196.4	366.	-1078.
156.00	-187.1	348.	-1015.
160.00	-178.5	332.	-959.
164.00	-170.5	317.	-907.
168.00	-163.1	303.	-860.
172.00	-156.1	290.	-817.
176.00	-149.5	279.	-778.
180.00	-143.4	268.	-742.
186.00	-134.9	253.	-693.
192.00	-127.1	239.	-650.
198.00	-119.9	227.	-611.
205.00	-112.2	214.	-570.
210.00	-107.2	206.	-545.
215.00	-102.4	198.	-521.
220.00	-97.9	191.	-499.
230.00	-89.8	178.	-459.
240.00	-82.4	166.	-425.
250.00	-75.9	156.	-396.
260.00	-69.9	147.	-369.
270.00	-64.5	139.	-346.
273.15	-62.9	136.	-340.
280.00	-59.6	132.	-326.
290.00	-55.1	125.	-308.
300.00	-51.0	119.	-291.
310.00	-47.2	113.	-276.
320.00	-43.7	108.	-263.
340.00	-37.4	100.	-239.
360.00	-31.9	92.	-219.
373.15	-28.7	87.	-207.
380.00	-27.1	85.	-202.
400.00	-22.9	80.	-187.
420.00	-19.1	75.	-175.
440.00	-15.8	70.	-163.
460.00	-12.7	66.	-153.
500.00	-7.5	59.	-137.
550.00	-2.2	52.	-120.
575.00	0.0	49.	-113.
600.00	2.0	47.	-107.
650.00	5.6	42.	-96.
700.00	8.5	38.	-88.
800.00	13.2	32.	-74.
900.00	16.7	28.	-64.
1000.00	19.5	24.	-56.
1100.00	21.6	21.	-50.
1300.00	24.8	17.	-40.
1500.00	27.0	14.	-34.

TABLE 6
SECOND VIRIAL COEFFICIENT OF XENON AND ITS TEMPERATURE DERIVATIVES

T K	B cm^3/mol	TdB/dT cm^3/mol	T^2d^2B/dT^2 cm^3/mol
220.00	-230.7	429.	-1225.
225.00	-221.2	411.	-1166.
230.00	-212.4	395.	-1111.
235.00	-204.0	380.	-1061.
240.00	-196.2	366.	-1015.
245.00	-188.7	353.	-972.
250.00	-181.7	341.	-933.
255.00	-175.1	329.	-896.
260.00	-168.8	319.	-861.
265.00	-162.8	308.	-829.
270.00	-157.2	299.	-799.
273.15	-153.7	293.	-781
280.00	-146.6	281.	-745.
290.00	-137.0	266.	-697.
300.00	-128.3	252.	-654.
310.00	-120.2	239.	-616.
320.00	-112.8	227.	-582.
330.00	-106.0	217.	-551.
340.00	-99.7	207.	-523.
350.00	-93.8	198.	-497.
360.00	-88.4	190.	-474.
370.00	-88.3	182.	-452
373.15	-81.7	180.	-446.
380.00	-78.5	175.	-433.
390.00	-74.0	169.	-415.
400.00	-69.8	163.	-398.
420.00	-62.2	152.	-368.
440.00	-55.4	142.	-342.
460.00	-49.2	133.	-319.
480.00	-43.7	126.	-299.
500.00	-38.8	119.	-282.
525.00	-33.1	111.	-262.
550.00	-28.1	104.	-245.
575.00	-23.6	98.	-230.
600.00	-19.6	93.	-215.
650.00	-12.5	84.	-193.
700.00	--6.6	76.	-175.
768.03	0.0	67.	-154.
800.00	2.7	64.	-146.
900.00	9.6	55.	-125.
1000.00	15.0	48.	-110.
1100.00	19.3	42.	-97.
1200.00	22.8	38.	-87.
1300.00	25.6	34.	-79.
1400.00	28.0	31.	-72.
1500.00	30.1	28.	-66.

TABLE 7
SECOND VIRIAL COEFFICIENT OF NITROGEN AND ITS TEMPERATURE DERIVATIVES

T K	B cm^3/mol	TdB/dT cm^3/mol	T^2d^2B/dT^2 cm^3/mol	T K	B cm^3/mol	TdB/dT cm^3/mol	T^2d^2B/dT^2 cm^3/mol
100.00	-160.0	304.	-874.	210.00	-31.1	94.	-224.
102.00	-154.1	293.	-837.	220.00	-26.9	88.	-209.
104.00	-148.5	283.	-802.	230.00	-23.2	82.	-195.
106.00	-143.2	273.	-769.	240.00	-19.7	78.	-183.
108.00	-138.2	264.	-739.	260.00	-13.8	70.	-163.
110.00	-133.4	256.	-711.	273.15	-10.5	65.	-152.
112.00	-128.7	248.	-684.	280.00	-8.9	63.	-147.
116.00	-120.4	233.	-637.	200.00	-4.7	58.	-134.
120.00	-112.7	220.	-594.	320.00	-1.2	53.	-122.
124.00	-105.7	208.	-557.	327.22	0.0	52.	-119.
128.00	-99.3	197.	-524.	340.00	1.9	49.	-113.
132.00	-93.4	188.	-494.	360.00	4.6	46.	-105.
136.00	-87.9	179.	-467.	373.15	6.2	44.	-100.
140.00	-82.8	171.	-442.	380.00	7.0	43.	-97.
144.00	-78.1	163.	-420.	400.00	9.1	40.	-91.
148.00	-73.7	156.	-400.	450.00	13.5	34.	-78.
152.00	-69.7	150.	-381.	500.00	16.8	30.	-68.
156.00	-65.8	144.	-364.	550.00	19.5	26.	-61.
160.00	-62.3	139.	-349.	600.00	21.7	24.	-54.
166.00	-57.3	131.	-327.	700.00	25.0	19.	-45.
172.00	-52.7	125.	-308.	800.00	27.3	16.	-38.
178.00	-48.6	118.	-291.	900.00	29.1	14.	-33.
184.00	-44.7	113.	-276.	1000.00	30.4	12.	-29.
190.00	-41.2	108.	-262.	1200.00	32.3	9.	-23.
200.00	35.9	100.	-242.	1400.00	33.5	7.	-19.

TABLE 8
SECOND VIRIAL COEFFICIENT OF OXYGEN AND ITS TEMPERATURE DERIVATIVES

T K	B cm^3/mol	TdB/dT cm^3/mol	T^2d^2B/dT^2 cm^3/mol	T K	B cm^3/mol	TdB/dT cm^3/mol	T^2d^2B/dT^2 cm^3/mol
100.00	-197.5	383.	-1201.	210.00	-44.8	104.	-259.
102.00	-190.1	367.	-1141.	220.00	-40.1	97.	-240.
104.00	-183.1	352.	-1087.	230.00	-35.9	91.	-223.
106.00	-176.5	339.	-1036.	240.00	-32.1	86.	-208.
108.00	-170.3	326.	-989.	250.00	-28.7	81.	-195.
110.00	-164.4	314.	-946.	260.00	-25.6	77.	-184.
112.00	-158.9	303.	-906.	273.15	-22.0	72.	-171.
114.00	-153.6	293.	-868.	280.00	-20.2	69.	-164.
116.00	-148.6	283.	-833.	300.00	-15.7	63.	-148.
120.00	-139.3	265.	-770.	320.00	-11.8	58.	-135.
124.00	-130.9	249.	-715.	340.00	-8.4	53.	-124.
128.00	-123.2	235.	-667.	360.00	-5.5	49.	-114.
132.00	-116.2	222.	-624.	373.15	-3.7	47.	-109.
136.00	-109.7	210.	-585.	380.00	-2.9	46.	-106.
140.00	-103.8	200.	-551.	400.00	-0.6	43.	-99.
144.00	-98.3	190.	-520.	405.88	0.0	42.	-97.
148.00	-93.2	182.	-492.	450.00	4.1	37.	-85.
154.00	-86.2	170.	-454.	500.00	7.7	32.	-74.
160.00	-79.9	159.	-422.	550.00	10.6	29.	-65.
166.00	-74.2	150.	-393.	600.00	12.9	25.	-58.
172.00	-69.1	142.	-368.	700.00	16.5	21.	-48.
178.00	-64.3	134.	-346.	800.00	19.1	18.	-41.
184.00	-60.0	127.	-326.	1000.00	22.4	13.	-31.
190.00	-56.0	121.	-308.	1200.00	24.5	10.	-25.
200.00	-50.0	112.	-281.	1400.00	25.9	8.	-20.

TABLE 9
SECOND VIRIAL COEFFICIENT OF DRY CO_2-FREE AIR AND ITS TEMPERATURE DERIVATIVES

T K	B cm^3/mol	TdB/dT cm^3/mol	T^2d^2B/dT^2 cm^3/mol	T K	B cm^3/mol	TdB/dT cm^3/mol	T^2d^2B/dT^2 cm^3/mol
100.00	-167.3	318.	-935.	210.00	-34.5	95.	-230.
102.00	-161.2	307.	-893.	220.00	-30.2	89.	-214.
104.00	-155.3	295.	-854.	230.00	-26.4	84.	-200.
106.00	-149.8	285.	-818.	240.00	-22.9	79.	-187.
108.00	-144.6	275.	-785.	250.00	-19.8	75.	-176.
110.00	-139.6	266.	-754.	260.00	-16.9	71.	-166.
112.00	-134.9	258.	-725.	273.15	-13.5	66.	-155.
114.00	-130.4	249.	-698.	280.00	-11.9	64.	-150.
116.00	-126.1	242.	-673.	300.00	-7.7	58.	-136.
118.00	-122.0	235.	-649.	320.00	-4.1	54.	-124.
120.00	-118.2	228.	-627.	340.00	-1.0	50.	-114.
124.00	-110.9	215.	-586.	346.81	0.0	48.	-111.
128.00	-104.3	204.	-550.	360.00	1.7	46.	-106.
132.00	-98.1	193.	-517.	373.15	3.4	44.	-101
136.00	-92.5	184.	-488.	380.00	4.2	43.	-98.
140.00	-87.3	176.	-462.	400.00	6.3	40.	-92.
144.00	-82.5	168.	-438.	450.00	10.7	35.	-79.
148.00	-78.0	161.	-416.	500.00	14.1	30.	-69
152.00	-73.8	154.	-396.	550.00	16.8	27.	-61.
156.00	-69.9	148.	-378.	600.00	19.0	24.	-55.
160.00	-66.2	142.	-361.	650.00	20.8	21.	-50.
166.00	-61.1	134.	-339.	700.00	22.3	19.	-45.
172.00	-56.5	127.	-319.	800.00	24.7	16.	-38.
178.00	-52.2	121.	-301.	900.00	26.4	14.	-33.
184.00	-48.3	115.	-284.	1000.00	27.8	12.	-29.
190.00	-44.7	110.	-270.	1200.00	29.7	9.	-23.
200.00	-39.3	102.	-248.	1400.00	30.9	7.	-19.

TABLE 10
SECOND VIRIAL COEFFICIENT OF HYDROGEN

T K	B cm^3/mol
24.00	-112.8
25.00	-106.2
26.00	-100.3
27.00	-94.8
28.00	-89.6
29.00	-85.0
30.00	-80.7
31.00	-76.7
32.00	-73.0
33.00	-69.5
34.00	-66.2
35.00	-63.2
36.00	-60.2
38.00	-55.0
40.00	-50.3
42.00	-46.2
44.00	-42.5
46.00	-39.2
48.00	-36.2
50.00	-33.4
54.00	-28.6
58.00	-24.5
62.00	-21.0
66.00	-17.9
70.00	-15.2
74.00	-12.9
78.00	-10.9
82.00	-8.9
86.00	-7.2
90.00	-5.7
100.00	-2.5
110.04	0.0
120.00	2.0
130.00	3.7
140.00	5.1
150.00	6.4
160.00	7.6
170.00	8.6
180.00	9.5
190.00	10.2
200.00	10.8
250.00	13.0
273.15	13.7
300.00	14.4
350.00	15.3
373.15	15.6
400.00	15.9
420.00	16.1

TABLE 11
SECOND VIRIAL COEFFICIENT OF DEUTERIUM

T K	B cm^3/mol
84.00	-10.4
88.00	-8.7
92.00	-7.0
96.00	-5.6
100.00	-4.2
110.00	-1.3
115.00	0.0
120.00	1.0
130.00	3.0
140.00	4.6
150.00	6.0
160.00	7.1
170.00	8.1
180.00	8.9
190.00	9.5
200.00	10.2
220.00	11.3
240.00	12.2
260.00	12.8
273.15	13.1
280.00	13.2
300.00	13.5
320.00	14.0
340.00	14.4
360.00	14.7
373.15	14.9
380.00	15.0
400.00	15.2
420.00	15.5

TABLE 12
SECOND VIRIAL COEFFICIENT OF WATER VAPOR (H_2O)

T K	B cm^3/mol
432.00	-311.2
434.00	-304.5
436.00	-298.1
438.00	-291.9
440.00	-285.5
442.00	-279.7
444.00	-273.9
446.00	-268.5
448.00	-263.2
450.00	-258.2
452.00	-253.4
454.00	-248.9
456.00	244.7
458.00	-240.5
460.00	-236.5
462.00	-232.6
464.00	-228.9
466.00	-225.4
468.00	-222.1
470.00	-218.5
475.00	-210.2
480.00	-202.5
485.00	-195.4
490.00	-188.6
495.00	-182.2
500.00	-176.2
505.00	-170.4
510.00	-165.0
515.00	-160.0
520.00	-155.3
530.00	-146.7
540.00	-139.1
550.00	-132.0
560.00	-125.3
570.00	-119.0
580.00	-113.1
590.00	-107.6
600.00	-102.5
610.00	-97.6
620.00	-93.0
630.00	-88.6
640.00	-84.4
650.00	-80.4
660.00	-76.6
670.00	-72.9
680.00	-69.4
690.00	-66.1
700.00	-62.9
710.00	-59.9
720.00	-57.0

TABLE 13
SECOND VIRIAL COEFFICIENT OF HEAVY WATER VAPOR (D_2O)

T K	B cm^3/mol
432.00	-314.5
434.00	-307.8
436.00	-301.3
438.00	-295.0
440.00	-288.6
442.00	-282.6
444.00	-276.9
446.00	-271.3
448.00	-265.9
450.00	-260.8
452.00	-255.9
454.00	-251.4
456.00	-247.0
458.00	-242.8
460.00	-238.8
462.00	-234.8
464.00	-231.1
466.00	-227.6
468.00	-224.2
470.00	-220.5
475.00	-212.2
480.00	-204.4
485.00	-197.2
490.00	-190.3
495.00	-183.8
500.00	-177.6
505.00	-171.8
510.00	-166.3
515.00	-161.1
520.00	-156.4
530.00	-147.7
540.00	-140.0
550.00	-132.8
560.00	-126.1
570.00	-119.6
580.00	-113.6
590.00	-108.1
600.00	-103.0
610.00	-98.0
620.00	-93.3
630.00	-88.8
640.00	-84.6
650.00	-80.6
660.00	-76.7
670.00	-73.1
680.00	-69.5
690.00	-66.2
700.00	-63.0
710.00	-59.9
720.00	-57.0

TABLE 14
SECOND VIRIAL COEFFICIENT OF CARBON DIOXIDE (CO_2)

T K	B cm^3/mol	T K	B cm^3/mol
250.00	-181.8	420.00	-52.6
255.00	-174.1	430.00	-49.1
260.00	-166.8	440.00	-45.9
265.00	-160.0	450.00	-42.8
270.00	-153.5	460.00	-40.0
273.15	-149.7	480.00	-34.7
275.00	-147.4	500.00	-30.0
280.00	-141.7	520.00	-25.8
285.00	-136.2	540.00	-21.9
290.00	-131.1	560.00	-18.4
295.00	-126.2	580.00	-15.3
300.00	-121.5	600.00	-12.4
310.00	-112.8	620.00	-9.8
320.00	-104.8	640.00	-7.4
330.00	-97.5	660.00	-5.1
340.00	-90.8	680.00	-3.1
350.00	-84.7	700.00	-1.3
360.00	-79.0	714.81	0.0
370.00	-73.8	750.00	2.7
373.15	-72.2	800.00	6.0
380.00	-68.9	850.00	8.8
390.00	-64.4	900.00	11.1
400.00	-60.2	950.00	13.0
410.00	-56.3	1000.00	14.6

TABLE 15
SECOND VIRIAL COEFFICIENT OF METHANE AND ITS TEMPERATURE DERIVATIVES

T K	B cm^3/mol	TdB/dT cm^3/mol	T^2d^2B/dT^2 cm^3/mol	T K	B cm^3/mol	TdB/dT cm^3/mol	T^2d^2B/dT^2 cm^3/mol
110.00	-334.0	671	-2244.	210.00	-95.3	193.	-505.
112.00	-322.2	643.	-2132.	220.00	-86.6	179	-463.
114.00	-311.0	618.	-2029.	230.00	-78.9	167.	-428
116.00	-300.5	594.	-1934.	240.00	-72.0	157.	-397.
118.00	-290.5	571.	-1846.	250.00	-65.8	147.	-369.
120.00	-281.1	550.	-1764.	260.00	-60.2	139.	-346.
122.00	-272.2	531.	-1688.	270.00	-55.2	131.	-324.
124.00	-263.7	512.	-1617.	273.15	-53.6	129.	-318.
126.00	-255.6	495.	-1551.	280.00	-50.5	124.	-306.
128.00	-248.0	479.	-1490.	290.00	-46.3	118.	-289.
130.00	-240.7	464.	-1432.	300.00	-42.3	113.	-273.
132.00	-233.7	449.	-1378.	320.00	-35.4	103.	-247.
134.00	-227.0	435.	-1327.	340.00	-29.4	94.	-225.
136.00	-220.7	422.	-1280.	360.00	-24.2	87.	-207.
140.00	-208.8	398.	-1193.	373.15	-21.2	83.	-196.
144.00	-197.9	377.	-1115	380.00	-19.7	81.	-191.
148.00	-187.8	357.	-1046.	400.00	-15.7	76.	-177.
152.00	-178.5	340.	-984.	450.00	-7.4	65.	-150.
156.00	-169.9	323.	-928.	500.00	-1.1	56.	-130.
160.00	-161.9	309.	-877.	509.66	0.0	55.	-126.
164.00	-154.5	295.	-831.	550.00	4.0	50.	-114.
168.00	-147.5	282.	-789.	600.00	8.1	45.	-102.
172.00	-141.0	271.	-751.	650.00	11.5	40.	-92.
176.00	-134.9	260.	-716.	700.00	14.3	37.	-83.
180.00	-129.2	250.	-683.	800.00	18.8	31.	-70.
184.00	-123.8	241.	-653.	900.00	22.1	26.	-61.
188.00	-118.7	232.	-626.	1000.00	24.7	23.	-53.
192.00	-113.9	224.	-600.	1100.00	26.8	20.	-47.
196.00	-109.4	216.	-576.	1300.00	29.8	16.	-39.
200.00	-105.1	209.	-554.	1500.00	31.9	13.	-32.

TABLE 16
THIRD VIRIAL COEFFICIENTS OF VARIOUS SUBSTANCES

C IN UNITS OF $10^2 cm^6/mol$

T K	He	Ne	Ar	Kr	Xe	N_2	O_2	Air	H_2	D_2	H_2O	D_2O	CO_2	CH_4
25									14.0					
30									16.0					
35									14.3					
40									12.1					
45									10.7					
50									9.6					
55									8.9					
60	2.7	4							8.4					
70	2.5	4							7.4					
80	2.4	4	7						6.9					
90	2.3	4	9						6.4					
100	2.2	4	12						6.1	6				
110	2.1	3	16						5.9	5				
120	2.0	3	20						5.7	5				
130	1.9	3	23						5.5	5				
140	1.8	3	25					28	5.4	5				
150	1.7	3	23					26	5.3	5				
160	1.6	3	22			26	23	24	5.2	5				
180	1.5	3	20			21	20	21	5.0	5				
200	1.3	3	18			19	17	19	4.8	5				
220	1.2	3	16	33		17	15	18	4.6	5				
240	1.1	3	15	30		16	13	17	4.5	5				
260	1.1	3	13	28		15	12	16	4.4	5				
273	1.1	3	12	27	62	15	11	15	4.2	5			57	29
280	1.0	3	12	26	59	15	11	15	4.1	5			56	28
300	1.0	2	11	24	54	14	10	15	3.9	5			52	26
320	1.0	2	11	23	50	14		14	3.6	5			49	24
340	0.9	2	10	21	46	14		14	3.4	5			45	22
360	0.8	2	9	20	41	13			3.2	5			42	21
380	0.8	2	9	19	36	13			3.0	4			38	19
400	0.7	2	9	18	34	13			2.9	4			36	18
420	0.7		9	18	32	12				3			32	17
440			8	17	30	12								16
460			8	16	28	12								16
480			8	16	26	12								15
500			7	15	24	12					-100	-150		15
525			7	15	22						-53	-64		14
550			7	14	20						-17	-20		14
575			7	14	18						+2	0		14
600			7	13							9	8		13
650				13							12	12		
700				12							10	12		

TABLE 17
BOYLE TEMPERATURE AND THE INVERSION TEMPERATURE OF VARIOUS SUBSTANCES

Substance	Boyle temperature	Inversion temperature
Helium	22.64	
Neon	122.11	231.42
Argon	411.52	779.91
Krypton	575.00	1089.72
Xenon	768.03	1455.79
Nitrogen	327.22	620.63
Oxygen	405.88	764.43
Air	346.81	658.79
Hydrogen	110.04	
Deuterium	115.30	
Carbon dioxide	714.81	
Methane	509.66	967.81

TABLE 18
POTENTIAL PARAMETERS FOR THE m - 6 POTENTIAL OF SELECTED SUBSTANCES

Substance	m	ε/k K	$b_o\ (= \frac{2\pi N}{3} c^{-3})$ cm^3/mol
Neon	18	47.74	22.83
Argon	18	160.87	43.74
Krypton	18	224.78	53.78
Xenon	18	300.29	73.32
Nitrogen	21	139.41	54.41
Oxygen	21	172.93	44.49
Air	21	147.76	50.95
Methane	21	217.14	57.96

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13. ABSTRACT

Tables of second virial coefficients as functions of temperature are presented for 14 gases. These gases are mainly noble gases and constituents of air. In most cases, these are based on a reexamination of the original P-V-T data. Where necessary and possible, these data have been refitted and improved experimental virials determined. In the case of eight of these gases, it has been possible to fit the experimental second virials to those predicted by the (m,6) potential function and potential parameters determined. In almost all cases, an optimum fit was obtained for m = 18. The optimum potential function was used for extrapolating the tables somewhat beyond the experimental range, and for obtaining temperature derivatives of B. In the case of the other six substances virial coefficients predicted by the (m,6) functions were used as a smoothing aid. Experimental third virial coefficients are presented at the experimental temperatures. A table of Boyle and Joule-Thomson inversion temperatures is also presented.

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14. KEY WORDS	LINK A		LINK B		LINK C	
	ROLE	WT	ROLE	WT	ROLE	WT
pressure						
volume						
temperature						
coefficients						
gas molecules						

AFSC
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