MODIFIED NUMERICAL TABLES FOR THE CALCULATION OF NON-SPHERICAL CONTRIBUTION TO SECOND VIRIAL COEFFICIENTS AND THE CORRELATION EQUATIONS OF STATE FOR CO_2, CS_2 AND C_6H_6

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Abstract

A revised analysis of the effect of long-range nonspherical terms in the intermolecular potential on the second virial coefficient is presented with a preferred Hartree-Fock-Dispersion functional (HFD-C) spherical core treatment of the integrations for small intermolecular distances. A set of modified numerical tables for the accurate calculation of the nonspherical contribution to the second virial coefficients is presented and a new correlation equation of $B_0^*(T^*)$ for CO_2, CS_2 and C_6H_6 is reported.

Introduction

The virial expansion of the equation of state of gases at low and moderate densities can be used to obtain information about intermolecular forces, in particular the second virial coefficient B(T) offers a convenient source of information on the intermolecular potential function.

The well-known statistical mechanical expression for the second virial coefficient is

$$B(T) = \frac{N_A}{2\Omega_0^2} \int_0^\infty r^2 dr \int \int [1-\exp(-U(r)/k_BT)] d\omega_1 d\omega_2 \tag{1}$$

where N_A is the Avogadro's number; k_B, the Boltzman constant; U(r), the intermolecular potential; ω, an an-

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gular variable determining the orientation of the molecule, and $\Omega = \int d\omega$. A standard method for the calculation of the second virial coefficients of nonspherical molecules is the perturbation scheme developed by Pople [1] and Buckingham [2], who represented the intermolecular potential as a spherically symmetric core plus a contribution due to the asphericity of the molecular charge distribution, such as interactions of dipole-dipole, quadrupole-quadrupole, and etc. so that

$$U(r) = U_0(r) + U_{ns}(r) \tag{2}$$

in which $U_0(r)$ depends only on the distance r between the molecular center of mass, and U_{ns} depends also on the angle ω, the relative orientation of the molecular pair. For the spherical symmetric part, Aziz and Chen [3] have proposed six models HFD-A, HFD-B, HFD-C, HFD-D, HFD-I, HFD-II which lead to better agreement between theoretical and experimental results. They preferred HFD-C in moderate and high temperatures upon comparison of theoretical and experimental results. On the other hand, the long-range orientational

part of molecular interactions can be expanded in a power series, i.e., a multipole expansion. This expression may be written explicitly in terms of tensorial interactions [4]. The corresponding expressions for the nonspherical contributions due to molecular interactions for two unlike axially symmetric molecules are summarized in the monograph of Mason and Spurling [5].

The nonspherical contribution to the second virial coefficient depends on the form assumed for the dominant spherical part and is usually expanded accordingly to produce an expression that gives corrections to the contribution in the form of series that converge rapidly for high temperatures. The coefficients of the series are integrals that are functions of the temperature, and are usually evaluated numerically and tabulated [6].

The main inadequacy of the above development is the form usually assumed for the long-range nonspherical terms in the potential, which is kept throughout the integrations even down to r= 0. In fact, the multipole expansion is not valid at small distances between molecules. Extension of the expressions for the long-range directional interactions into the region of small distances between molecular centers leads to values of the parameters which are not uniquely defined. The formulas are convergent for high temperatures, but the point is that it is at the high temperatures that effects occurring at small intermolecular separations might be expected to be most important.

In this paper, we use a convenient function $G_n(r)$ in such a way that the usual long-range nonspherical interactions are modified and the effects of short-range interactions can be used for calculation of the integrals $<r^{-n}>$ involved in the nonspherical contribution to the second virial coefficient.

Our results are presented as a set of improved tables for the accurate calculation of the nonspherical contributions to the second virial coefficients. The results are qualitatively similar to the previous work [7], but the function defined in this paper produces more effect on the final virial coefficient than does the previous paper.

Furthermore, the reduced spherical part of the second virial coefficient $B_0^*(T^*)$ can be constructed by first calculating the contributions $B_{ns}(T)$, subtracting the calculated $B_{ns}(T)$ from experimental $B(T)$, and then reducing with two scaling parameters σ and ε. However, we conclude that the correlation equations of the functional $B_0^*(T^*)$ for several nonspherical molecules presented earlier [8], which did not include any convenient function $G_n(r)$, do not need to be revised except for CO_2, because the higher-order terms in the

additive contribution arising from the quadrupole interactions are not negligible in this case. As a result, a new correlation equation of $B_0^*(T^*)$ for CO_2 is presented. Next, we apply the method to calculate the second virial coefficients of CS_2 and C_6H_6 and present the correlation equations of functional $B_0^*(T^*)$ for these two molecules.

Calculations

If two nonspherical molecules interact, the potential energy will depend on the relative spatial orientations of the molecules as well as on the distance apart. The intermolecular pair potential can be obtained from Equation 2. We suggest that the expression for the orientational potential can be modified in conjunction with a controlling function

$$G_n(r) \equiv \exp\left[-n\left(\frac{r_m}{r}-1\right)^2\right] \qquad r < r_m$$

$$G_n(r) \equiv 1 \qquad\qquad r > r_m \qquad (3)$$

where r_m is the position of the potential minimum. Therefore, we write the intermolecular pair potential (2) as

$$U(r) = U_0(r) + U_{ns}(r).\,G_n(r) \qquad (4)$$

The perturbation expansion for the second virial coefficient then becomes

$$B^*(T^*) = B_0^*(T^*) + B_{ns}^*(T^*) \qquad (5)$$

where

$$T^* \equiv k_B T/\varepsilon \qquad (6)$$

$$B^* \equiv B/b \quad , \qquad b \equiv \frac{2}{3}\pi N_A \sigma^3 \qquad (7)$$

Here ε and σ stand for the depth of the potential well and the value of r for which $U_0(r) = 0$, respectively. The nonspherical contribution to the second virial coefficient, B_{ns}^*, can be written as [6]

$$
\begin{aligned}
B_{ns}^*(T^*) = \ & B_{ns}^*(\mu\mu) + B_{ns}^*(\mu\theta) + B_{ns}^*(\theta\theta) + B_{ns}^*(\mu,\text{ind}\mu) + \\
& + B_{ns}^*(\mu\theta,\text{ind}\mu) + B_{ns}^*(\theta,\text{ind}\mu) + B_{ns}^*(\mu,\text{ind}\theta) + B_{ns}^*(C_6\text{anis}) \\
& + B_{ns}^*(\mu\times\theta) + B_{ns}^*(\mu,\text{ind}\mu\times\theta,\text{ind}\mu) + \\
& + B_{ns}^*(\mu\mu\times\mu,\text{ind}\mu) + B_{ns}^*(\mu\mu\times\theta,\text{ind}\mu) + \\
& + B_{ns}^*(\theta\theta\times C_6\text{anis}) + B_{ns}^*(\mu,\text{ind}\mu\times C_6\text{anis}) + \\
& + B_{ns}^*(\theta\times\text{ind}\mu\times C_6\text{anis}) + B_{ns}^*(\text{shape}) \qquad (8)
\end{aligned}
$$

where

$$B_{ns}^{*}((\mu\mu) = -\frac{2}{3}(\frac{\mu^{*2}}{T^*})^2 [I_6 + \frac{1}{25}(\frac{\mu^{*2}}{T^*})^2 I_{12} + ...] \qquad (9\text{-}A)$$

$$B_{ns}^{*}(\mu\theta) = -\frac{6}{5}(\frac{\mu^*\theta^*}{T^*})^2 [I_8 + \frac{726}{3185}(\frac{\mu^*\theta^*}{T^*})^2 I_{16} + ...] \qquad (9\text{-}B)$$

$$B_{ns}^{*}(\theta\theta) = -\frac{6}{5}(\frac{\theta^{*2}}{T^*})^2 [I_{10} - \frac{6}{49}(\frac{\theta^{*2}}{T^*}) I_{15} + ...] \qquad (9\text{-}C)$$

$$B_{ns}^{*}(\mu, \text{ind}\mu) = -\frac{2}{15}(\frac{\mu^{*2}\alpha_d^*}{T^*})^2 [I_{12} + 11\alpha_d^{*2} I_{18}] + ... \qquad (9\text{-}D)$$

$$B_{ns}^{*}(\mu\theta, \text{ind}\mu) = -\frac{864}{77}(\frac{\mu^*\theta^*\alpha_d^*}{T^*})^2 [I_{14} + ... \qquad (9\text{-}E)$$

$$B_{ns}^{*}(\theta, \text{ind}\mu) = -\frac{162}{455}(\frac{\theta^{*2}\alpha_d^*}{T^*})^2 [I_{16} + ... \qquad (9\text{-}F)$$

$$B_{ns}^{*}(\mu, \text{ind}\theta) = -\frac{162}{455}(\frac{\mu^{*2}\alpha_q^*}{T^*})^2 [I_{16} + ... \qquad (9\text{-}G)$$

$$B_{ns}^{*}(C_6 \text{ anis}) = -\frac{2}{15}(\frac{\kappa C_6^*}{T^*})^2 (1+\frac{19}{10}\kappa^2) I_{12} + ... \qquad (9\text{-}H)$$

$$B_{ns}^{*}(\mu\times\theta) = \frac{3}{5}(\frac{\mu^*\theta^*}{T^*})^2 [(\frac{\mu^{*2}}{T^*}) I_{11} + \frac{24}{11}(\frac{\theta^{*2}}{T^*}) I_{13} + ... \qquad (9\text{-}I)$$

$$B_{ns}^{*}(\mu, \text{ind}\mu\times\theta, \text{ind}\mu) = -\frac{144}{385}(\frac{\mu^*\theta^*\alpha_d^*}{T^*})^2 I_{14} + ... \qquad (9\text{-}J)$$

$$B_{ns}^{*}(\mu\mu\times\mu, \text{ind}\mu) = -\frac{4}{3}(\frac{\mu^{*2}}{T^*})^2\alpha_d^* I_{12} [\alpha_d^* + \frac{1}{15}(\frac{\mu^{*2}}{T^*}) + ...] \qquad (9\text{-}K)$$

$$B_{ns}^{*}(\mu\mu\times\theta, \text{ind}\mu) = -\frac{48}{385}(\frac{\mu^{*2}}{T^*})^2 (\frac{\theta^{*2}}{T^*})\alpha_d^* I_{14} + ... \qquad (9\text{-}L)$$

$$B_{ns}^{*}(\theta\theta\times C_6 \text{ anis}) = \frac{27}{25}(\frac{\theta^{*2}}{T^*})(\frac{C_6^*}{T^*})\kappa^2 I_{11} + ... \qquad (9\text{-}M)$$

Table I. Values of dimensionless integrals $I_n(T^*)$ as shown in Equation (10)

T^*	I_6	I_7	I_8	I_9	I_{10}
0.5	1.7672	1.9599	2.0893	2.1724	2.2213
0.6	1.3997	1.5354	1.6268	1.6861	1.7218
0.7	1.1950	1.2999	1.3711	1.4180	1.4472
0.8	1.0672	1.1534	1.2125	1.2522	1.2778
0.9	0.9809	1.0548	1.1062	1.1415	1.1652
1.0	0.9194	0.9848	1.0310	1.0634	1.0860
1.2	0.8386	0.8934	0.9333	0.9628	0.9848
1.4	0.7888	0.8376	0.8744	0.9027	0.9251
1.6	0.7559	0.8011	0.8362	0.8644	0.8875
1.8	0.7329	0.7759	0.8103	0.8388	0.8631
2.0	0.7163	0.7580	0.7922	0.8213	0.8469
2.5	0.6909	0.7315	0.7665	0.7979	0.8269
3.0	0.6779	0.7188	0.7556	0.7897	0.8222
3.5	0.6710	0.7131	0.7520	0.7889	0.8248
4.0	0.6677	0.7112	0.7522	0.7920	0.8312
4.5	0.6664	0.7115	0.7548	0.7973	0.8397
5.0	0.6664	0.7132	0.7587	0.8038	0.8492
6.0	0.6688	0.7190	0.7687	0.8188	0.8699
7.0	0.6727	0.7262	0.7799	0.8346	0.8908
8.0	0.6773	0.7339	0.7913	0.8503	0.9114
9.0	0.6822	0.7418	0.8027	0.8656	0.9311
10.0	0.6871	0.7495	0.8137	0.8803	0.9499

Table I. Continued

T*	I_{11}	I_{12}	I_{13}	I_{14}	I_{15}
0.5	2.2454	2.2499	2.2404	2.2206	2.1932
0.6	1.7401	1.7456	1.7415	1.7304	1.7142
0.7	1.4633	1.4698	1.4693	1.4636	1.4541
0.8	1.2934	1.3011	1.3032	1.3013	1.2963
0.9	1.1804	1.1893	1.1937	1.1948	1.1934
1.0	1.1018	1.1119	1.1182	1.1217	1.1232
1.2	1.0014	1.0139	1.0237	1.0313	1.0376
1.4	0.9432	0.9581	0.9708	0.9819	0.9921
1.6	0.9072	0.9244	0.9399	0.9542	0.9677
1.8	0.8845	0.9039	0.9219	0.9390	0.9557
2.0	0.8701	0.8916	0.9120	0.9319	0.9514
2.5	0.8544	0.8809	0.9070	0.9331	0.9593
3.0	0.8538	0.8851	0.9164	0.9481	0.9804
3.5	0.8604	0.8960	0.9322	0.9691	1.0071
4.0	0.8705	0.9103	0.9510	0.9929	1.0362
4.5	0.8825	0.9263	0.9713	1.0178	1.0661
5.0	0.8955	0.9430	0.9921	1.0430	1.0961
6.0	0.9224	0.9769	1.0335	1.0927	1.1547
7.0	0.9492	1.0099	1.0735	1.1402	1.2104
8.0	0.9750	1.0416	1.1115	1.1852	1.2629
9.0	0.9996	1.0716	1.1474	1.2275	1.3122
10.0	1.0230	1.0999	1.1813	1.2673	1.3586

Table I. Continued

T*	I_{16}	I_{17}	I_{18}	I_{19}	I_{20}
0.5	2.1602	2.1236	2.0843	2.0434	2.0016
0.6	1.6943	1.6718	1.6476	1.6222	1.5962
0.7	1.4418	1.4276	1.4122	1.3959	1.3792
0.8	1.2892	1.2807	1.2713	1.2612	1.2507
0.9	1.1904	1.1861	1.1811	1.1756	1.1699
1.0	1.1233	1.1225	1.1210	1.1193	1.1173
1.2	1.0429	1.0475	1.0518	1.0559	1.0601
1.4	1.0015	1.0106	1.0195	1.0285	1.0376
1.6	1.9808	0.9938	1.0068	1.0200	1.0334
1.8	0.9722	0.9887	1.0054	1.0224	1.0399
2.0	0.9710	0.9908	1.0109	1.0316	1.0528
2.5	0.9860	1.0133	1.0414	1.0704	1.1005
3.0	1.0136	1.0478	1.0832	1.1199	1.1582
3.5	1.0463	1.0870	1.1292	1.1733	1.2193
4.0	1.0811	1.1279	1.1766	1.2276	1.2810
4.5	1.1164	1.1690	1.2240	1.2816	1.3421
5.0	1.1516	1.2096	1.2706	1.3346	1.4019
6.0	1.2198	1.2882	1.3603	1.4363	1.5166
7.0	1.2843	1.3624	1.4448	1.5320	1.6242
8.0	1.3450	1.4319	1.5240	1.6216	1.7251
9.0	1.4020	1.4971	1.5982	1.7054	1.8195
10.0	1.4554	1.5583	1.6677	1.7841	1.9080

Table I. Continued

T*	L_{21}	L_{22}	L_{23}	L_{24}	L_{25}
0.5	1.9595	1.9175	1.8758	1.8349	1.7948
0.6	1.5700	1.5438	1.5180	1.4925	1.4676
0.7	1.3623	1.3455	1.3289	1.3126	1.2968
0.8	1.2402	1.2297	1.2194	1.2095	1.1999
0.9	1.1641	1.1585	1.1530	1.1478	1.1430
1.0	1.1154	1.1136	1.1121	1.1109	1.1100
1.2	1.0643	1.0688	1.0737	1.0789	1.0845
1.4	1.0469	1.0567	1.0668	1.0775	1.0887
1.6	1.0473	1.0617	1.0766	1.0922	.1.1085
1.8	1.0579	1.0766	1.0960	1.1162	1.1373
2.0	1.0748	1.0976	1.1213	1.1459	1.1716
2.5	1.1317	1.1641	1.1979	1.2331	1.2699
3.0	1.1980	1.2395	1.2829	1.3283	1.3758
3.5	1.2673	1.3176	1.3702	1.4254	1.4833
4.0	1.3369	1.3956	1.4572	1.5219	1.5900
4.5	1.4056	1.4724	1.5427	1.6167	1.6946
5.0	1.4727	1.5474	1.6260	1.7090	1.7966
6.0	1.6013	1.6909	1.7856	1.8858	1.9918
7.0	1.7220	1.8255	1.9353	2.0517	2.1752
8.0	1.8349	1.9516	2.0755	2.2073	2.3473
9.0	1.9407	2.0697	2.2070	2.3532	2.5088
10.0	2.0400	2.1806	2.3304	2.4902	2.6606

Table I. Continued

T*	L_{26}	L_{27}	L_{28}	L_{29}	L_{30}
0.5	1.7557	1.7177	1.6809	1.6453	1.6109
0.6	1.4434	1.4200	1.3973	1.3754	1.3544
0.7	1.2815	1.2667	1.2526	1.2391	1.2262
0.8	1.1908	1.1821	1.1740	1.1664	1.1593
0.9	1.1386	1.1347	1.1313	1.1283	1.1259
1.0	1.1096	1.1096	1.1101	1.1111	1.1127
1.2	1.0907	1.0973	1.1045	1.1123	1.1207
1.4	1.1005	1.1129	1.1260	1.1398	1.1544
1.6	1.1255	1.1433	1.1619	1.1814	1.2018
1.8	1.1592	1.1822	1.2061	1.2311	1.2573
2.0	1.1984	1.2263	1.2555	1.2859	1.3177
2.5	1.3083	1.3484	1.3904	1.4343	1.4802
3.0	1.4255	1.4775	1.5321	1.5893	1.6492
3.5	1.5441	1.6078	1.6748	1.7452	1.8191
4.0	1.6615	1.7368	1.8160	1.8995	1.9873
4.5	1.7767	1.8632	1.9545	2.0508	2.1524
5.0	1.8890	1.9866	2.0897	2.1986	2.3138
6.0	2.1041	2.2230	2.3490	2.4825	2.6240
7.0	2.3063	2.4455	2.5933	2.7503	2.9170
8.0	2.4962	2.5546	2.8232	3.0025	3.1933
9.0	2.6746	2.8512	3.0394	3.2399	3.4537
10.0	2.8423	2.0361	3.2429	3.4636	3.6991

Table II. Nonspherical contributions, B_{ns} (cm^3/mol), for gases as a function of temperature. Values of force parameters for N_2, O_2, CO, NO, N_2O, C_2H_4 C_2H_6 and CO_2 are given in Ref. 8 and for CS_2 and C_6H_6 in Ref. 11.

T K or °C	N_2	O_2	CO	NO	N_2O
100K	-3.8004	-------	-35.0401	-------	-------
150	-1.4276	-1.2205	-13.4387	-6.0383	-------
200	-0.7584	-0.6301	-7.2059	-3.0963	-------
250	-0.4765	-0.3905	-4.5509	-1.9036	-------
300	-0.3304	-0.2689	-3.1646	-1.3002	-6.7086
0°C	-0.3983	-0.3252	-3.8100	-1.5792	-8.4812
20	-0.3459	-0.2817	-3.3119	-1.3636	-7.1028
40	-0.3035	-0.2467	-2.9093	-1.1908	-6.0403
60	-0.2689	-0.2182	-2.5789	-1.0501	-5.2040
80	-0.2400	-0.1947	-2.3041	-0.9340	-4.5337
100	-0.2158	-0.1749	-2.0728	-0.8368	-3.9882
150	-0.1697	-0.1375	-1.6321	-0.6533	-2.9972
200	-0.1375	-0.1114	-0.3231	-0.5261	-2.3428
250	-0.1140	-0.0924	-1.0974	-0.4340	-1.8872
300	-0.0962	-0.0782	-0.9270	-0.3651	-1.5566
350	-0.0825	-0.0671	-0.7949	-0.3119	-1.3087
400	-0.0716	-0.0584	-0.6903	-0.2701	-1.1177
450	-0.0629	-0.0513	-0.6059	-0.2364	-0.9673
500	-0.0557	-0.0455	-0.5367	-0.2090	-0.8465
600	-0.0447	-0.0367	-0.4307	-0.1671	-0.6663
700	-0.0368	-0.0303	-0.3544	-0.1371	-0.5401
800	-------	-0.0255	-0.2473	-0.1148	-0.4479
900	-------	-0.0218	-0.2534	-0.0977	-0.3784
1000	-------	-------	-0.2087	-0.0796	-0.3245
1500	-------	-------	-------	-------	-0.1762
2000	-------	-------	-------	-------	-0.1123

$$B_{ns}^*(\mu, ind\mu \times C_6\, anis) = -\frac{4}{15}\left(\frac{\mu^{*2}}{T^*}\right)\left(\frac{C_6^*}{T^*}\right)\alpha_d^* \kappa I_{12} + \dots \text{(9-N)}$$

$$B_{ns}^*(\theta, ind\mu \times C_6 anis) = -\frac{144}{385}\left(\frac{\theta^{*2}}{T^*}\right)\left(\frac{C_6^*}{T^*}\right)\alpha_d^* \kappa I_{14} + \dots$$

$$\text{(9-O)}$$

$$B_{ns}^*(shape) = \frac{384}{75}\left(\frac{\kappa D}{T^{*2}}\right)I_8 + \frac{192}{133}\frac{D}{T^*}\left(\frac{\theta^{*2}}{T^*}\right)I_{22} - \frac{384}{105}\left(\frac{D}{T^*}\right)^2 I_{14} + \dots$$

$$\text{(9-P)}$$

Results and Discussion

The dimensionless integrals $I_n(T^*)$ that appear in the expressions for the various contributions to B_{ns}^* are defined as

$$I_n(T^*) \equiv \frac{n-3}{2}(\sigma/r_m)^{n-3}\int \int^\infty \frac{dx}{x^{n-2}}G_n(x)\exp(-U_0^*/T^*) \quad (10)$$

where $x = r/r_m$ and $U_0^*(X) = U_0/\varepsilon$. The form chosen for U_0 is the HFD-C potential used by Aziz and Chen [3]. Values of $I_n(T^*)$ were calculated by numerical integration and are given in Table I, for $0.5 < T^* < 10$ and $0 < n < 30$. The nonspherical contribution, $B_{ns}(T)$, can be obtained by Equations 8-9. The numerical values of $B_{ns}(T)$ for ten gases are given in Table II. Notice that all the values $B_{ns}(T)$ are small with respect to the values of $B_0(T)$.

By subtraction of the calculated $B_{ns}(T)$ from the experimental values of $B(T)$ and reduction with σ and ε, the functional $B_0^*(T^*)$ is obtained. Selected experimental data are taken from the critical survey of Dymond and Smith [9]. In this work, the functional $B_0^*(T^*)$ is assumed to have the same form as that of the noble gases [10], but obviously the numerical values of its coefficients differ. According to previous works, the reduced functional $B_0^*(T^*)$ for the noble gases and

Table II. Continued

T K or °C	C_2H_4	C_2H_6	CS_2	CO_2	C_6H_6
250K	-1.9178	-0.1393	-19.0566	-35.6454	-84.2375
300	-1.2171	-0.0886	-10.3537	-22.8867	-57.5663
0°C	-1.5323	-0.1115	-14.0675	-28.6559	-69.6691
20	-1.2874	-0.0937	-11.1508	-24.1762	-60.2819
40	-1.0979	-0.0800	-9.4138	-20.6910	-52.9234
60	-0.9483	-0.0692	-7.4715	-17.9254	-47.0301
80	-0.8281	-0.0605	-6.2746	-15.6932	-42.2225
100	-0.7301	-0.0533	-5.3426	-13.8648	-38.2384
150	-0.5514	-0.0404	-3.7539	-10.5128	-30.7781
200	-0.4328	-0.0318	-2.7850	-8.2742	-25.6247
250	-0.3499	-0.0257	-2.1520	-6.7016	-21.0756
300	-0.2895	-0.0213	-1.7161	-5.5522	-19.0373
350	-0.2441	-0.0180	-1.4032	-4.6851	-16.8199
400	-0.2090	-0.0154	-1.1708	-4.0136	-15.0433
450	-0.1813	-0.0134	-0.9934	-3.4823	-13.5898
500	-0.1590	-0.0118	-0.8548	-3.0541	-12.3796
600	-0.1256	-0.0093	-0.6548	-2.4126	-10.4825
700	-0.1021	-0.0076	-0.5199	-1.9608	-9.0650
800	-0.0850	-0.0063	-0.4243	-1.6296	-7.9670
900	-0.0720	-0.0054	-0.3539	-1.3790	-7.0920
1000	-0.0618	-0.0046	-0.3004	-1.1843	-6.3785
1500	-0.0339	-0.0026	-0.1584	-0.6451	-4.1684
2000	-0.0270	-0.0017	-0.0999	-0.4119	-3.0280

⊠ Michels (1935)
+ Cottrell (1956)
* Mac Cormak (1950)
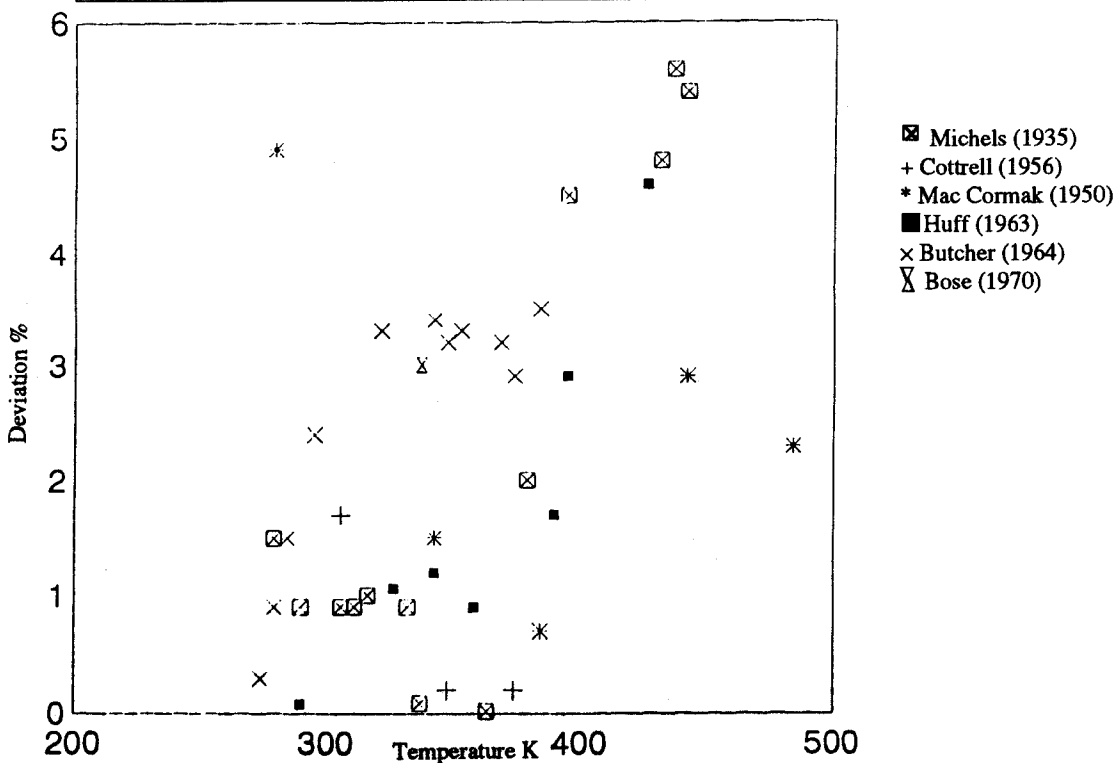■ Huff (1963)
× Butcher (1964)
� Bose (1970)

Figure I. Deviation plot for the second virial coefficient of CO_2. Selected experimental data are taken from Ref. 9.
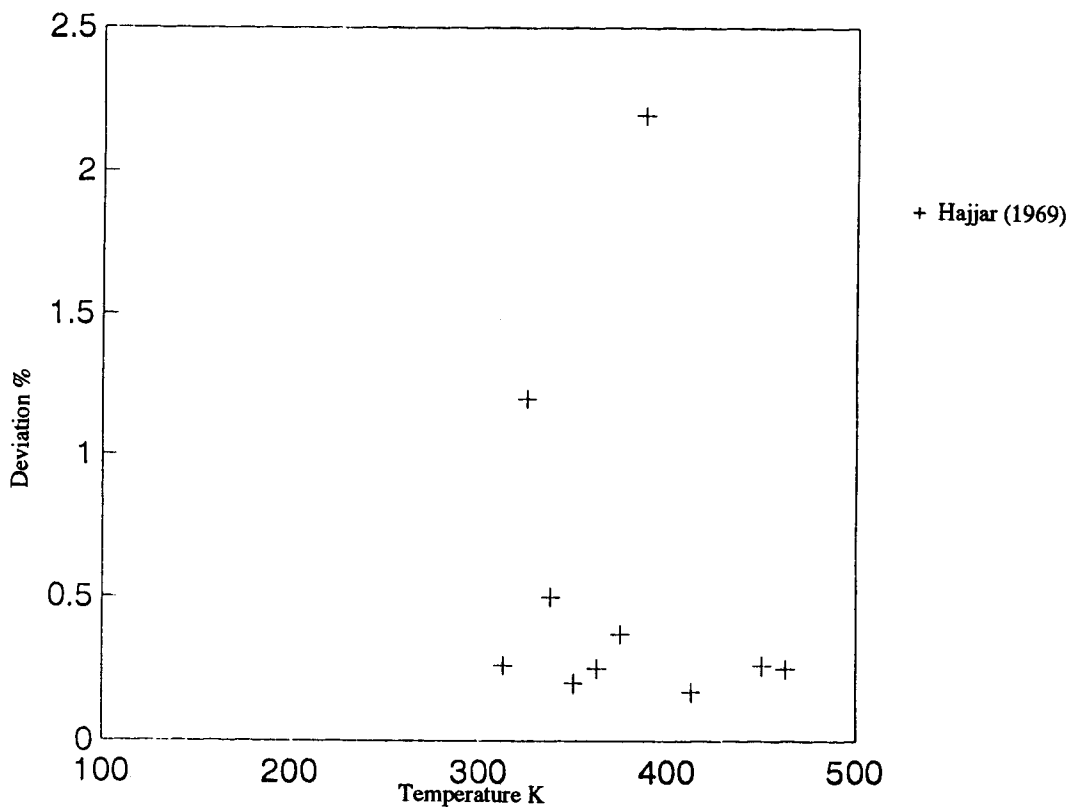
Figure II. Deviation plot for the second virial coefficient of CS_2. Selected experimental data are taken from Ref. 9.
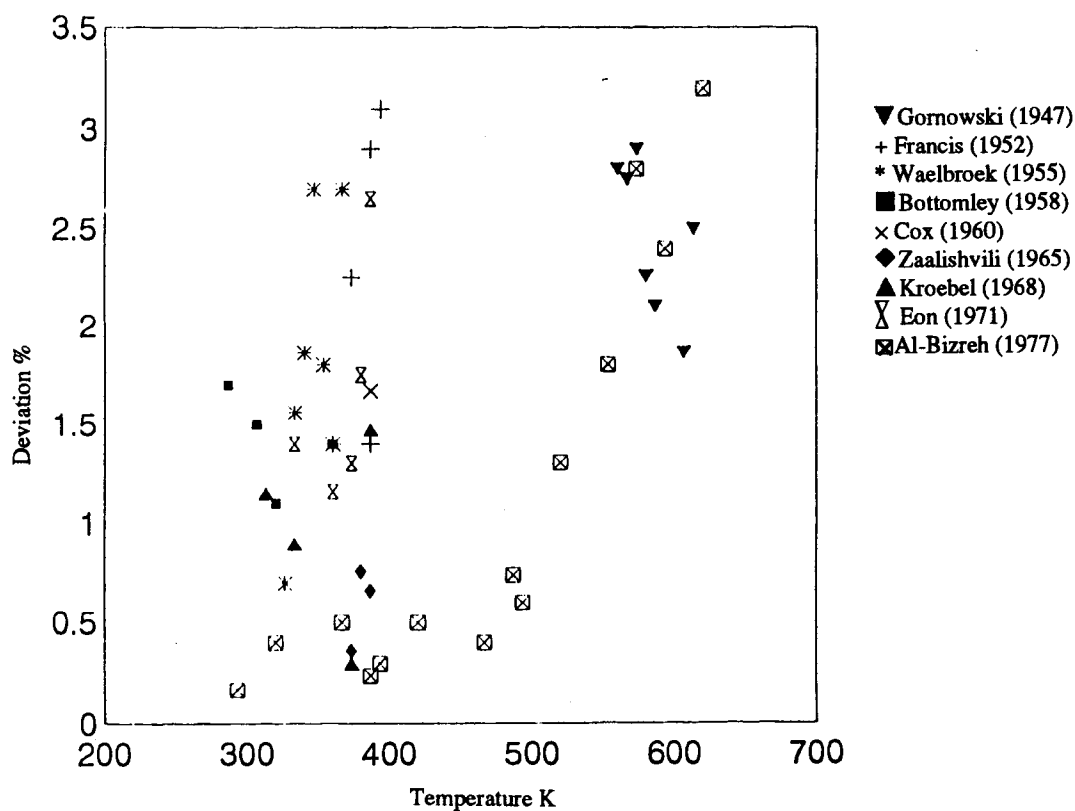

Figure III. Deviation plot for the second virial coefficient of C_6H_6. Selected experimental data are taken from Ref. 9.

Table III. Coefficients of Equation (11) for computation of the functional B_0^*.

	C_0	C_1	C_2	C_3	C_4
CO_2	0.77088	-0.62868	-1.76645	2.65872	-1.02333
CS_2	0.51066	-1.62814	6.86488	37.87559	61.93789
C_6H_6	1.32777	-2.63948	2.67594	-1.92352	0.85792

for several polyatomic gases in the region $1 < T^* < 10$ is in the form

$$B_0^*(T^*) = -T^* e^{1/T^*}[C_0 + C_1 \ln T^* + C_2 (\ln T^*)^2 + C_3 (\ln T^*)^3 + C_4 (\ln T^*)^4]. \tag{11}$$

Comparison of the new correlation with an earlier correlation shows that the correlation equations of the functionals $B_0^*(T^*)$, obtained in this work, are very close to those in the previous correlation equations, except for CO_2 because the quadrupole-quadrupole interactions are not negligible in this molecule. A new correlation equation for CO_2 is obtained and the correlation equations for CS_2 and C_6H_6, which heretofore have not been reported, are also calculated. The coefficients C_n of Equation 11 for the computation of B_0^* of CO_2, CS_2 and C_6H_6 are given in Table III. The calculated second virial coefficients are compared in Figures I-III with experimental data.

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