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Second Virial Coefficients of Axially Symmetric Molecules

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The paper presents a contribution to the second virial coefficient due to the asphericity of the molecular charge distribution. This contribution is conveniently divided into terms representing the classical electrostatic interaction between the two charge distributions, the anisotropy of dispersion forces, and the shape of the molecular core. These are considered quantitatively. Results from recalculating the nonspherical contributions to the second virial coefficients with a good spherical core are obtained from statistical mechanics and applied to the CO_2 gas. Explilcit formulas are given for the simple cases of axially symmetric molecules.

The potential energy between two polyatomic molecules is usually assumed to consist of a spherically symmetric component plus a contribution due to the asphericallly of the molecular charge distribution. A method of integration for B(T) developed by Pople[1] viewed the orientation-dependent parts of the potential as perturbations on the central-force part. Later the applications to various polar gases were worked out in some detail by Buckingham and Pople.[2] Using Orcutt's method, reasonable values of molecular quadrupole moments could be obtained even by neglecting the effect of the shape component (i.e., the anisotropy of the repulsive part of the potential) on the second virial coefficient.[3]

Spurling and Mason obtained the parameters of the spherical component of the potential from the viscosity data, then, used in conjunction with second virial coefficient data, determined the quadrupole moments and "shape" parameters of the molecules.[4] It was found that one could get rid of the effect of the quadrupole moment on viscosity by simply assigning sligthly different values of ε_0 and σ_0 and using Najafi's correlation curve for the viscosity.[5,6]

The greatest virtue of the virial equation of state lies in the direct relation of the virial coefficients to the intermolecular forces. We provide a quantitative discussion of some of these forces and obtain corresponding expressions for the second virial coefficients. Here, results of recalculating the nonspherial contributions to the second virial coefficients with a spherical core, similar to that used by Boushehri, et al.,[7] are obtained from statistical mechanics and applied to a polyatomic gas.

Calculation

An indirect procedure is usually used to determine intermolecular forces from virial coefficients due to the failure of the direct approach. Many kinetic theory transport properties (viscosity, heat conductivity, ordinary diffusion) depend primarily on the fact that a force exists between molecules, and only secondarily on the nature of the force. But whether the force is one of attraction or repulsion can be an essential point for the virial coefficients, whose very sign depends on the nature of force.

It should be mentioned that while much progress in describing the thermodynamic properties of assemblies of molecules with spherical symmetry has been made, there are many molecules whose force fields depend on relative orientation. The potential model for the calculation of the second virial coefficients may be written as.[7]

$$V(r) = V_o(\text{spherical}) + V(\mu\mu) + V(\mu\theta) + V(\theta\theta) + V(\mu, \text{ind}\mu) + V(\mu\theta, \text{ind}\mu) + V(\theta, \text{ind}\mu) + V(C_6\,\text{anis}) + V(\text{shape}) \quad (1)$$

where

$$V(\mu\mu) = -\frac{\mu^2}{r^3}(2C_1C_2 - S_1S_2C), \quad (2\text{-a})$$

$$V(\mu\theta) = \frac{3\mu\theta}{2r^4}(C_2 - C_1)(3C_1C_2 - 2S_1S_2C + 1), \quad (2\text{-b})$$

$$V(\theta\theta) = \frac{3\theta^2}{4r^5}[1 - 5C_1^2 - 5C_2^2 - 15C_1^2C_2^2 + 2(4C_1C_2 - S_1S_2C)^2], \quad (2\text{-c})$$

$$V(\mu, \text{ind}\mu) = -\frac{\mu^2\bar{\alpha}}{2r^6}(3C_1^2 + 3C_2^2 - 2) - \frac{\mu^2\bar{\alpha}^2}{r^9}(8C_1C_2 - S_1S_2C), \quad (2\text{-d})$$

$$V(\mu\theta, \text{ind}\mu) = -\frac{12\mu\theta\bar{\alpha}}{r^7}(C_1^3 + C_2^3), \quad (2\text{-e})$$

$$V(\theta, \text{ind}\mu) = -\frac{9\theta^2\bar{\alpha}}{8r^8}(4C_1^4 + 4C_2^4 + S_1^4 + S_2^4 - \frac{8}{3}), \quad (2\text{-f})$$

$$V(C_6\,\text{anis}) = \frac{KC_6}{r^6}[1 - \frac{3}{2}(1 - K)(C_1^2 + C_2^2) - \frac{3}{2}K(2C_1C_2 - S_1S_2C)^2]. \quad (2\text{-g})$$

The simplest force field reproducing the orientation effect of the shape of an axially symmetric nonspherical molecule is

$$V(\text{shape}) = \frac{A}{r^n}(3C_1^2 + 3C_2^2 - 2), \quad (2\text{-h})$$

where A is a constant and n is an integer (usually 12). There is no particular theoretical basis for the form of V(shape). The average polarizability $\bar{\alpha}$ is given by $\bar{\alpha}=(\alpha^{11}+2\alpha^{\perp})/3$ and the anisotropy K is defined by $K=(\alpha^{11}-2\alpha^{\perp})/3\bar{\alpha}$, where α^{11} is the polarizability along the axis of symmetry and $\alpha^{\perp}$ that perpendicular to it. The quadrupole moment θ is defined by

$$\theta=\sum_i e_i(Z_i^2-X_i^2)$$

where e_i is the ith element of charge and Z_i and X_i are its coordinates in a system where Z axis is the symmetry axis and the origin is the center of mass. The angle-dependent abbreviations used in Eq. 2 are

$$C_1=\cos\theta_1,\ C_2=\cos\theta_2,\ S_1=\sin\theta_1,\ S_2=\sin\theta_2,$$
$$\text{and } C=\cos\phi.$$

Here θ_1, θ_2, and ϕ are the usual angles describing the mutual orientation of two linear molecules.

The nonspherical contribution to the second virial coefficient, ΔB^*, is obtained using a good spherical core (HFD-I) given in Table 1 of Ref. 8. In conjunction with this model and in terms of the dimensionless quantities $T^*=T/(\varepsilon_o/k)$, $B^*=B/(2\pi N_A\sigma_o^3/3)$, $\mu^*=\mu/(\varepsilon_o\sigma_o^3)^{1/2}$, $\theta^*=\theta/(\varepsilon_o\sigma_o^5)^{1/2}$, $\alpha^*=\bar{\alpha}/\sigma_o^3$, and $C_6^*=C_6/\varepsilon_o\sigma_o^6$

$$\begin{aligned}\Delta B^* = {} & B^*(\mu\mu)+B^*(\mu\theta)+B^*(\theta\theta)+B^*(\mu,\text{ ind}\mu)\\ & +B^*(\mu\theta,\text{ ind}\mu)+B^*(\theta,\text{ ind}\mu)+B^*(C_6\text{ anis})\\ & +B^*(\mu X\theta)+B^*(\mu,\text{ ind}\mu\ X\theta,\text{ ind}\mu)\\ & +B^*(\mu\mu X\mu,\text{ ind}\mu)+B^*(\mu\mu X\theta,\text{ ind}\mu)\\ & +B^*(\theta\theta X\ C_6\text{ anis})+B^*(\mu,\text{ ind}\mu\ X\ C_6\text{ anis})\\ & +B^*(\theta,\text{ ind}\mu\ X\ C_6)\text{ anis}).\end{aligned}\tag{3}$$

Where

$$B^*(\mu\mu)=-\frac{2}{3}\left(\frac{\mu^{*2}}{T^*}\right)^2\left[J_6+\frac{1}{25}\left(\frac{\mu^{*2}}{T^*}\right)^2J_{12}+\cdots\right]\tag{4-a}$$

$$B^*(\mu\theta)=-\frac{6}{5}\left(\frac{\mu^*\theta^*}{T^*}\right)^2\left[J_8+0.22794\left(\frac{\mu^*\theta^*}{T^*}\right)^2J_{16}+\cdots\right]\tag{4-b}$$

$$B^*(\theta\theta)=-\frac{6}{5}\left(\frac{\theta^{*2}}{T^*}\right)^2\left[J_{10}-\frac{6}{49}\left(\frac{\theta^{*2}}{T^*}\right)J_{15}+\cdots\right]\tag{4-c}$$

$$B^*(\mu,\text{ ind}\mu)=-\frac{2}{15}\left(\frac{\mu^{*2}\alpha^*}{T^*}\right)^2\left[J_{12}+11\alpha^{*2}J_{18}+\cdots\right]\tag{4-d}$$

$$B^*(\mu\theta,\text{ ind}\mu)=-\frac{864}{77}\left(\frac{\mu^*\theta^*\alpha^*}{T^*}\right)^2J_{14}+\cdots\tag{4-e}$$

$$B^*(\theta,\text{ ind}\mu)=-\frac{162}{455}\left(\frac{\theta^{*2}\alpha^*}{T^*}\right)^2J_{16}+\cdots\tag{4-f}$$

$$B^*(C_6\text{ anis})=-\frac{2}{15}\left(\frac{K\,C_6^*}{T^*}\right)^2\left(1+\frac{19}{10}K^2\right)J_{12}+\cdots\tag{4-g}$$

$$B^*(\mu X\theta)=\frac{3}{5}\left(\frac{\mu^*\theta^*}{T^*}\right)^2\left[\left(\frac{\mu^{*2}}{T^*}\right)J_{11}+\frac{24}{35}\left(\frac{\theta^{*2}}{T^*}\right)J_{13}+\cdots\right]\tag{4-h}$$

$$B^*(\mu,\text{ ind}\mu X\theta,\text{ ind}\mu)=-\frac{144}{385}\left(\frac{\mu^*\theta^*\alpha^*}{T^{*2}}\right)^2J_{14}+\cdots\tag{4-i}$$

$$B^*(\mu\mu X\mu,\text{ ind}\mu)=-\frac{4}{3}\left(\frac{\mu^{*2}}{T^*}\right)^2\alpha^*J_{12}\left(\alpha^*+\frac{1}{15}\left(\frac{\mu^{*2}}{T^*}\right)\right)+\cdots\tag{4-j}$$

$$B^*(\mu\mu X\theta,\text{ ind}\mu)=-\frac{48}{385}\left(\frac{\mu^{*2}}{T^*}\right)^2\left(\frac{\theta^{*2}}{T^*}\right)\alpha^*J_{14}+\cdots\tag{4-k}$$

$$B^*(\theta\theta X\ C_6\text{ anis})=\frac{27}{25}\left(\frac{\theta^{*2}}{T^*}\right)\left(\frac{C_6^*}{T^*}\right)K^2J_{11}+\cdots\tag{4-l}$$

Table 1. Various Contributions to the Second Virial Coefficient of CO_2 as Calculated by Eq. 3

T^*	$B^*(\theta\theta)$	$B^*(\theta,\text{ ind}\mu)$	$B^*(\theta\theta X C_6\text{anis})$	$B^*(C_6\text{anis})$
0.8969	−0.835640	−0.000653	0.132884	−0.041282
1.1135	−0.490684	−0.000487	0.076886	−0.024025
1.8345	−0.160320	−0.000288	0.024759	−0.007882
2.7313	−0.072695	−0.000217	0.011244	−0.003649
3.5874	−0.043746	−0.000188	0.006810	−0.002245
4.4843	−0.029393	−0.000171	0.004612	−0.001541
T^*	$B^*(\theta,\text{ ind}\mu X C_6\text{anis})$	B_o^*(spherical)	$B_{\text{theo.}}^*$	$B_{\text{expt.}}^{*\,a)}$
0.8969	−0.005654	−2.5329	−3.283245	−3.6755
1.1135	−0.003338	−1.6923	−2.133948	−2.2420
1.8345	−0.001143	−0.5483	−0.693174	−0.6338
2.7313	−0.000552	−0.0664	−0.132269	−0.0578
3.5874	−0.000351	0.1431	0.103380	0.1570
4.4843	−0.000248	0.2668	0.240059	0.2680

$\sigma_o=3.769$ Å, $\varepsilon_o/k=245.3$ K (Ref. 10)
$\bar{\alpha}=2.63$ Å^3 $K=0.2664$ (Ref. 11)
$\theta=4.3\times10^{-26}$ esu (Ref. 12)
$C_6=158.7$ hatree (Bohr)^6 (Ref. 14)
$B_{\text{theo.}}=B_o^*(\text{spherical})+\Delta B^*$
a) $B_{\text{expt.}}^*$(smoothed values) (Ref. 13)

Table 2. Functions $J_n(T^*)$ for the Calculation of Nonspherical Contributions to Second Virial Coefficients Obtained by HFD-I Potential

T^*	J_6	J_7	J_8	J_9	J_{10}	J_{11}	J_{12}	J_{13}	J_{14}
0.5	1.7885	1.9875	2.1238	2.2146	2.2721	2.3052	2.3203	2.3222	2.3145
0.6	1.4178	1.5595	1.6577	1.7246	1.7688	1.7966	1.8125	1.8197	1.8208
0.7	1.2115	1.3223	1.4004	1.4550	1.4929	1.5188	1.5361	1.5473	1.5542
0.8	1.0828	1.1750	1.2412	1.2889	1.3237	1.3492	1.3682	1.3827	1.3942
0.9	0.9961	1.0762	1.1349	1.1786	1.2119	1.2378	1.2587	1.2762	1.2916
1.0	0.9344	1.0063	1.0601	1.1014	1.1341	1.1609	1.1837	1.2041	1.2230
1.2	0.8538	0.9156	0.9640	1.0032	1.0364	1.0658	1.0927	1.1185	1.1439
1.4	0.8046	0.8611	0.9071	0.9462	0.9811	1.0135	1.0447	1.0758	1.1074
1.6	0.7724	0.8259	0.8712	0.9113	0.9485	0.9842	1.0198	1.0560	1.0936
1.8	0.7503	0.8024	0.8478	0.8895	0.9292	0.9685	1.0084	1.0498	1.0933
2.0	0.7346	0.7861	0.8324	0.8759	0.9184	0.9613	1.0056	1.0522	1.1017
2.5	0.7118	0.7640	0.8136	0.8626	0.9126	0.9649	1.0203	1.0800	1.1446
3.0	0.7015	0.7561	0.8099	0.8650	0.9228	0.9845	1.0513	1.1242	1.2043
3.5	0.6974	0.7551	0.8137	0.8751	0.9408	1.0121	1.0903	1.1767	1.2727
4.0	0.6969	0.7580	0.8215	0.8893	0.9629	1.0438	1.1336	1.2337	1.3460
4.5	0.6985	0.7632	0.8317	0.9059	0.9874	1.0780	1.1794	1.2935	1.4225
5.0	0.7013	0.7698	0.8433	0.9238	1.0133	1.1135	1.2266	1.3549	1.5010
6.0	0.7093	0.7853	0.8687	0.9618	1.0670	1.1866	1.3235	1.4808	1.6622
7.0	0.7188	0.8022	0.8953	1.0009	1.1217	1.2607	1.4217	1.6088	1.8269
8.0	0.7290	0.8196	0.9223	1.0401	1.1763	1.3349	1.5203	1.7379	1.9942
9.0	0.7394	0.8370	0.9491	1.0789	1.2306	1.4086	1.6187	1.8676	2.1633
10.0	0.7497	0.8543	0.9755	1.1172	1.2841	1.4818	1.7169	1.9977	2.3340

T^*	J_{15}	J_{16}	J_{17}	J_{18}	J_{19}	J_{20}	J_{21}	J_{22}	J_{23}
0.5	2.3001	2.2808	2.2584	2.2340	2.2086	2.1829	2.1574	2.1325	2.1086
0.6	1.8176	1.8114	1.8035	1.7946	1.7853	1.7762	1.7676	1.7598	1.7530
0.7	1.5582	1.5605	1.5618	1.5627	1.5638	1.5653	1.5677	1.5711	1.5758
0.8	1.4037	1.4123	1.4205	1.4288	1.4376	1.4473	1.4581	1.4702	1.4839
0.9	1.3058	1.3195	1.3334	1.3478	1.3631	1.3797	1.3977	1.4174	1.4390
1.0	1.2414	1.2597	1.2787	1.2985	1.3197	1.3425	1.3671	1.3938	1.4227
1.2	1.1697	1.1965	1.2245	1.2544	1.2863	1.3207	1.3577	1.3978	1.4412
1.4	1.1402	1.1747	1.2114	1.2507	1.2930	1.3387	1.3881	1.4417	1.4998
1.6	1.1332	1.1754	1.2206	1.2693	1.3220	1.3792	1.4413	1.5089	1.5825
1.8	1.1397	1.1895	1.2433	1.3016	1.3650	1.4340	1.5094	1.5917	1.6818
2.0	1.1549	1.2125	1.2749	1.3430	1.4173	1.4988	1.5880	1.6860	1.7937
2.5	1.2152	1.2925	1.3775	1.4713	1.5749	1.6896	1.8168	1.9580	2.1150
3.0	1.2928	1.3909	1.4999	1.6214	1.7570	1.9087	2.0786	2.2692	2.4834
3.5	1.3798	1.4996	1.6341	1.7853	1.9557	2.1481	2.3656	2.6120	2.8916
4.0	1.4724	1.6150	1.7764	1.9594	2.1674	2.4042	2.6744	2.9831	3.3366
4.5	1.5688	1.7352	1.9249	2.1418	2.3902	2.6752	3.0030	3.3806	3.8165
5.0	1.6679	1.8590	2.0786	2.3313	2.6228	2.9598	3.3502	3.8035	4.3307
6.0	1.8721	2.1155	2.3988	2.7290	3.1150	3.5672	4.0982	4.7230	5.4599
7.0	2.0822	2.3816	2.7339	3.1494	3.6406	4.2229	4.9148	5.7389	6.7229
8.0	2.2970	2.6559	3.0823	3.5905	4.1977	4.9251	5.7986	6.8504	8.1201
9.0	2.5159	2.9375	3.4432	4.0515	4.7851	5.6725	6.7486	8.0572	9.6526
10.0	2.7384	3.2261	3.8159	4.5315	5.4021	6.4645	7.7644	9.3595	11.3221

T^*	J_{24}	J_{25}	J_{26}	J_{27}	J_{28}	J_{29}	J_{30}
0.5	2.0859	2.0647	2.0449	2.0268	2.0105	1.9959	1.9831
0.6	1.7475	1.7434	1.7407	1.7396	1.7402	1.7426	1.7467
0.7	1.5819	1.5895	1.5988	1.6098	1.6228	1.6377	1.6546
0.8	1.4992	1.5164	1.5356	1.5569	1.5805	1.6064	1.6348
0.9	1.4626	1.4885	1.5168	1.5476	1.5812	1.6177	1.6574
1.0	1.4542	1.4884	1.5255	1.5658	1.6094	1.6567	1.7078
1.2	1.4882	1.5391	1.5942	1.6539	1.7187	1.7888	1.8647

Table 2. (Countinued)

T^*	J_{24}	J_{25}	J_{26}	J_{27}	J_{28}	J_{29}	J_{30}
1.4	1.5628	1.6313	1.7058	1.7867	1.8746	1.9703	2.0745
1.6	1.6627	1.7502	1.8457	1.9500	2.0640	2.1886	2.3249
1.8	1.7805	1.8886	2.0072	2.1374	2.2804	2.4376	2.6107
2.0	1.9122	2.0427	2.1866	2.3454	2.5207	2.7146	2.9291
2.5	2.2898	2.4846	2.7019	2.9448	3.2165	3.5208	3.8621
3.0	2.7244	2.9960	3.3026	3.6490	4.0411	4.4856	4.9902
3.5	3.2094	3.5711	3.9836	4.4546	4.9934	5.6108	6.3192
4.0	3.7419	4.2077	4.7437	5.3617	6.0755	6.9014	7.8586
4.5	4.3207	4.9049	5.5831	6.3719	7.2910	8.3640	9.6190
5.0	4.9452	5.6628	6.5026	7.4873	8.6442	10.0059	11.6120
6.0	6.3309	7.3627	8.5876	10.0449	11.7823	13.8581	16.3434
7.0	7.9004	9.3128	11.0110	13.0575	15.5291	18.5211	22.1508
8.0	9.6565	11.5203	13.7867	16.5495	19.9253	24.0599	29.1355
9.0	11.6028	13.9928	16.9294	20.5464	25.0127	30.5413	37.4012
10.0	13.7434	16.7387	20.4538	25.0738	30.8337	38.0330	47.0540

Table 3. The $B_o^*(T^*)$ for the Calculation of Spherical Contributions to Second Virial Coefficients

T^*	$B_o^*(T^*)$	T^*	$B_o^*(T^*)$	T^*	$B_o^*(T^*)$
0.30	−24.8221	1.50	−0.9123	3.40	0.1078
0.35	−16.5478	1.55	−0.8457	3.50	0.1272
0.40	−12.0793	1.60	−0.7841	3.60	0.1454
0.45	−9.3485	1.65	−0.7270	3.70	0.1624
0.50	−7.5309	1.70	−0.6738	3.80	0.1783
0.55	−6.2440	1.75	−0.6244	3.90	0.1933
0.60	−5.2895	1.80	−0.5781	4.00	0.2075
0.65	−4.5557	1.85	−0.5349	4.10	0.2208
0.70	−3.9752	1.90	−0.4943	4.20	0.2333
0.75	−3.5053	1.95	−0.4562	4.30	0.2452
0.80	−3.1174	2.00	−0.4203	4.40	0.2564
0.85	−2.7922	2.10	−0.3546	4.50	0.2670
0.90	−2.5158	2.20	−0.2958	4.60	0.2771
0.95	−2.2781	2.30	−0.2430	4.70	0.2867
1.00	−2.0716	2.40	−0.1954	4.80	0.2958
1.05	−1.8906	2.50	−0.1521	4.90	0.3044
1.10	−1.7307	2.60	−0.1127	5.00	0.3126
1.15	−1.5885	2.70	−0.0767	6.00	0.3768
1.20	−1.4613	2.80	−0.0437	7.00	0.4188
1.25	−1.3468	2.90	−0.0133	8.00	0.4476
1.30	−1.2432	3.00	0.0147	9.00	0.4679
1.35	−1.1491	3.10	0.0406	10.00	0.4826
1.40	−1.0632	3.20	0.0646	20.00	0.5189
1.45	−0.9846	3.30	0.0870	30.00	0.5084

$$B^*(\mu, \text{ ind}\mu X\ C_6 \text{ anis}) = -\frac{4}{15}\left(\frac{\mu^{*2}}{T^*}\right)\left(\frac{C_6^*}{T^*}\right)\alpha^* K J_{12} + \cdots \quad (4\text{-m})$$

$$B^*(\theta, \text{ ind}\mu X\ C_6 \text{ anis}) = -\frac{144}{385}\left(\frac{\theta^{*2}}{T^*}\right)\left(\frac{C_6^*}{T^*}\right)\alpha^* K J_{14} + \cdots \quad (4\text{-n})$$

Here

$$J_n(T^*) \equiv \frac{n-3}{2}\int_0^\infty \frac{dr^*}{(r^*)^{n-2}} \exp\left(-V_o^*/T^*\right)$$

where $V_o^* \equiv V_o/\varepsilon_o$ and $r^* \equiv r/\sigma_o$

The $J_n(T^*)$s are functions tabulated in Table 2 and B_o^* (spherical) are given in Table 3. Boushehri et al. have tabulated $J_n(T^*)$ using (HFD-C) given by Aziz and Chen[8] for n=6 through 30 and for T^* from 0.5 to 10.0.[7] In Ref. 9 results for molecules with octupole moments have also been discussed.

Results and Discussion

Various contributions to B(T) for CO_2 calculated according to Eq. 3 are given in Table 1. The scaling parameters for CO_2 are taken from Ref. 10. Comparison of present work and experimental value of CO_2 are also shown in Table 1.

It should be mentioned that in Ref. 7 the J_n integrals for the nonspherical contributions were calculated for

the HFD-C potential while in the present paper they are calculated for the HFD-I potential.

In Ref. 7, a set of J_n tables is justified by the argument that the values will be insensitive to the details of the potential. Comparison of the new J_n tables with the earlier J_n tables confirms this observation.

References

1) J. A. Pople, *Proc. R. Soc. London, Ser. A*, **221**, 508 (1954).
2) A. D. Buckingham and J. A. Pople, *Trans. Faraday Soc.*, **51**, 1173 (1955).
3) R. H. Orcutt, *J. Chem. Phys.*, **39**, 605 (1963).
4) T. H. Spurling and E. A. Mason, *J. Chem. Phys.*, **46**, 322 (1967).
5) B. Najafi, E. A. Mason, and J. Kestin, *Physica*, **119A**, 387 (1983).
6) A. Boushehri, *J. Phys. Chem. Ref. Data.*, (Submitted).
7) A. Boushehri, E. A. Mason, and J. Kestin, Intern. *J. Thermophys.*, **7**, 1115 (1986).
8) R. A. Aziz and H. H. Chen, *J. Chem. Phys.*, **67**, 5719 (1977).
9) S. Kielich, *Physica.*, **28**, 511 (1962).
10) J. Kestin and S. T. Ro, *Ber. Bunsenges. Phys. Chem.*, **86**, 948 (1982).
11) N. J. Bridge and A. D. Buckingham, *Proc. R. Soc. London, Ser. A*, **295**, 334 (1966).
12) A. D. Buckingham, R. L. Disch, and D. A. Dummur, *J. Am. Chem. Soc.*, **90**, 3104 (1968).
13) J. H. Dymond and E. B. Smith, "The Virial Coefficients of Pure Gases and Mixtures," Oxford University Press, London (1980).
14) B. L. Jhanwar and W. J. Meath, *Chem. Phys.*, **67**, 185 (1982).