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The Second Virial Coefficient of 3-Center *Lennard-Jones* Molecules and Its Relation to 1- and 2- Center Molecules*

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The second virial coefficients of homonuclear three-center *Lennard-Jones* molecules are calculated with various parameters of the isosceles triangle connecting the three sites. A special effort is made to establish the reduced *Boyle* temperatures T_B and the values of the second virial coefficients at $T/T_B = 0.3$ for the sake of comparison with one- and two-center *Lennard-Jones* molecules. It is shown that it is possible to find parameter values of the interaction potential of one- and two-center *Lennard-Jones* molecules which give very similar values of second virial coefficients for $T/T_B \geqslant 0.3$, and the equivalence conditions are established. These conditions might not only give a basis for a microscopic scaling of state variables, but also some restrictions for the validity of the group contribution concept.

(Keywords: Second virial coefficient; Three-center Lennard-Jones molecules; Corresponding states)

Der Zweite Virialkoeffizient von Drei-Zentren Lennard-Jones Molekülen und seine Beziehung zu dem von Ein-Zentren und Zwei-Zentren Molekülen

Es wird der zweite Virialkoeffizient homonuklearer Drei-Zentren *Lennard-Jones* Moleküle angegeben, und zwar für verschiedene Parameter des gleichschenkligen Dreiecks, welches die Zentren verbindet. Besonderes Gewicht ist auf die Ausrechnung der reduzierten *Boyle*-Temperatur T_B und auf die Werte des zweiten Virialkoeffizienten bei $T/T_B = 0.3$ gelegt, welche zum Vergleich mit Ein- und Zwei-Zentren *Lennard-Jones* Molekülen herangezogen werden. Es wird gezeigt, daß für Ein- und Zwei-Zentren *Lennard-Jones* Moleküle Parameter des Wechselwirkungspotentials gefunden werden können, welche sehr ähnliche Werte

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für die zweiten Virialkoeffizienten für Temperaturen $T/T_B \geqslant 0.3$ ergeben; diese Äquivalenzbeziehungen werden angegeben. Diese Bedingungen geben einerseits einen Hinweis auf die mikroskopische Skalierung der Zustandsvariablen, andererseits deuten sie auf Gültigkeitsgrenzen des Gruppenbeitrags-Konzepts.

Introduction

In a recent paper, *Kohler* and *Quirke*[1] gave values for the second virial coefficients of 2-center *Lennard-Jones* molecules and compared them to those of an 1-center molecule. Values of second virial coefficients of 2-center *Lennard-Jones* molecules have appeared in the meantime also in the monograph of *Maitland* et al.[2].

The question raised in the paper of *Kohler* and *Quirke*[1] is the following: For 1-center *Lennard-Jones* (1 C*LJ*) molecules, the potential parameters ε and σ (minimum and zero of the potential) provide a microscopic scaling of the state variables as do the critical parameters T_c, p_c, v_c on a macroscopic basis. E.g., the following relations hold approximately

$$kT_c/\varepsilon = 1.26, \tag{1}$$

$$p_c\sigma^3/\varepsilon = 0.117, \tag{2}$$

$$v_c/N_A\sigma^3 = 3.11, \tag{3}$$

and we have exactly

$$kT_B/\varepsilon = 3.418, \tag{4}$$

where T_B is the *Boyle* temperature (zero of the second virial coefficient); k is the *Boltzmann* constant and N_A *Avogadro*'s number.

A 2-center *Lennard-Jones* (2 C*LJ*) molecule is characterized by the parameters ε and σ of the site-site potential and by the distance l between sites, which is frequently expressed in a reduced way $L = l/\sigma$. How have the relations (1)–(4) to be modified for 2 C*LJ* molecules as function of the elongation L?

As *Kohler* and *Quirke* noted, an immediate answer is possible for equ. (4), and it has been given in graphical form (cf. Fig. 1). As far as equ. (1) is concerned, *Kohler* and *Quirke* suggested an empirical relationship

$$\left(\frac{T_c}{T_B}\right)_{2\mathrm{C}LJ} = \left(\frac{T_C}{T_B}\right)_{1\mathrm{C}LJ}(1 + aL), \tag{5}$$

with $a = 0.15$. Later, *Fischer* et al.[3] calculated critical points by perturbation theory for 1- and 2-center *Lennard-Jones* molecules. In view of the shortcomings of perturbation theory around critical densities they called the calculated values "pseudocritical points". From their pseudocritical points, one can derive the following values for the parameter a:

0.148 ($L = 0.3292$), 0.166 ($L = 0.505$), 0.158 ($L = 0.670$), 0.145 ($L = 0.793$) in good agreement with the postulate of *Kohler* and *Quirke*.

Equ. (5) shows, that substitution of an ε_{2CLJ}-value by an "effective" ε_{1CLJ} would differ whether made for the *Boyle* temperature (vanishing density) or the critical temperature (medium density). The same is true if an "effective" σ_{1CLJ}-value is sought for a 2 *CLJ* molecule. The value for the "effective" σ_{1CLJ} would be different if determined for the saturation density, the critical density or the low density region (second virial coefficients). The following procedure has been suggested by *Kohler* and *Quirke* to arrive at "effective" σ_{1CLJ}-values for 2 *CLJ* molecules valid at low densities:

1. Find the second virial coefficient B for an 1 *CLJ* at $T/T_B = 0.3$, and find B for a 2 *CLJ* again at $T/T_B = 0.3$. The value of $(B/\sigma^3)_{2CLJ}$, $T/T_B = 0.3$ will be the more negative, the bigger the elongation L.
2. The "effective" σ_{1CLJ}-value $\sigma_{1,\mathrm{eff}}$ is then obtained from the relation

$$\frac{B_{1CLJ}}{\sigma^3_{1,\mathrm{eff}}} = \left(\frac{B}{\sigma^3}\right)_{2CLJ}, \quad T/T_B = 0.3 \tag{6}$$

The choice of $T/T_B = 0.3$ is arbitrary. It is about the lowest reduced temperature, up to which the whole curves of virial coefficients for different L can be made almost identical to $B_{1CLJ}/\sigma^3_{1,\mathrm{eff}}$ by a proper choice of $\sigma_{1,\mathrm{eff}}$. At lower reduced temperature, $(B/\sigma^3)_{2CLJ}$ is the more negative than $B_{1CLJ}/\sigma^3_{1,\mathrm{eff}}$ the bigger the elongation L. A similar statement has been made recently by *Kerl* and *Häusler*[4], who could correlate the second virial coefficients of a number of molecules such that they came on the same curve between T_B and T_C but showed a spread of curves at temperatures below T_C.

The form of $\sigma_{1,\mathrm{eff}}$ as function of L resembles much the graph of kT_B/ε as function of L.

The purpose of the present paper is to extend the findings on 2 *CLJ* molecules to 3-center *Lennard-Jones* molecules (3 *CLJ*).

Results

Characteristics of 3 *CLJ*

We will restrict ourselves to homonuclear 3 *CLJ*, and correspondingly to isosceles triangles. Instead of the angle, we will use the ratio of height h to longest side l, h/l, as one parameter, and the reduced length of the longest side $L = l/\sigma$, as the other, besides ε and σ of the *LJ* site-site potential. The full pair potential u between two 3 *CLJ* molecules consists of nine site-site interactions, which depend on the distance r between center of mass and the mutual orientation. For a linear 3 *CLJ* ($h/l = 0$) the mutual orientation is determined by three angles θ_1, θ_2, φ, where θ_i is the angle between the axis of molecule i and the connecting line of centers of mass, and φ says how much molecule 2 is turned out of plane formed by the axis of molecule 1 and the connecting line of centers of mass. For a non-linear 3 *CLJ*, we need two additional angles ψ_1, ψ_2 to describe all mutural orientations. One may visualize this as follows: Specify one molecular axis, e.g. the height of the triangle. Then the angles θ_1, θ_2, φ are needed to characterize the mutual orientation of the axes. The angles ψ_1 and ψ_2 give then the rotation of the molecules 1 and 2 around the specified axis.

The second virial coefficient is, therefore, given by

$$B(T) = -2\pi N_A \int_0^{\infty} \int_{-1}^{+1} \int_{-1}^{+1} \int_0^{2\pi} \int_0^{\pi} \int_0^{\pi} (e^{-u/kT} - 1)\, d\psi_1\, d\psi_2\, d\varphi\, d\cos\theta_1\, d\cos\theta_2\, r^2\, dr \tag{7}$$

Calculations

Due to the sixfold integration the straightforward numerical method—construction of a sufficient number of grid points and application of *Simpson*'s rule—is inappropriate. One value of B would take hours on a fast computer.

The method followed in this paper is a procedure of sampling the variables independently at random, with subsequent smoothing of the density of points along the r-axis.

It might be of interest to compare this method with a method tried in our most recent work[5], where the integration over the angular variables followed the work of *Conroy*[6], but the integration over r was done by *Simpson*'s rule. As Table 1 shows, this last method is more accurate but takes longer than the random sampling procedure.

Table 1. *Comparison of the various calculation methods for second virial coefficients given by six-dimensional integrals*

Method	Grid Points, *Simpson*'s Rule	Random Sampling Procedure	*Conroy*-Method for Angles, *Simpson*'s Rule for Distance
No. of Configurations	$2 \cdot 10^8$	$4 \cdot 10^5$	$8 \cdot 10^5$
Statistical Error	0.01%	0.1–0.5%[b]	0.01%
Systematic Error[a]	0.1%	0.5–1.5%[b]	0.1%

[a] Estimates based on comparisons of integrals of lower dimensionality.

[b] The biggest errors occur for linear or near-linear molecules with large elongation.

The main purpose of this work was to calculate *Boyle*-temperatures and second virial coefficients at $T/T_B = 0.3$, but one calculation for model propane was done over the whole temperature interval. Table 2 summarizes all results.

Fig. 1 shows the variation of the *Boyle*-temperature as function of the elongation of the long side L in comparison to the united atom, for which

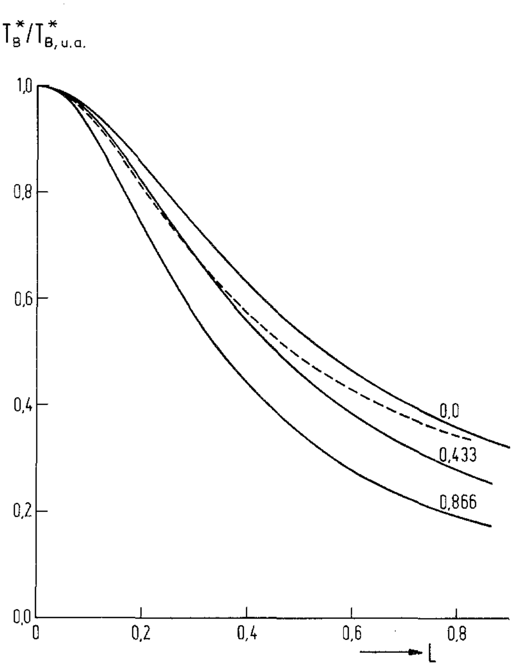

Fig. 1. The reduced *Boyle* temperature, $T_B^* = kT_B/\varepsilon$, of the 3 *CLJ*, relative to the reduced *Boyle* temperature of the united atom, $T_B^* = 30.761$, as function of the reduced length of the long side of the isosceles triangle, $L = l/\sigma$. The parameters refer to the relative height of the triangle, $h/l = 0.0$ means linear 3 *CLJ*, $h/l = 0.866$ means equilateral triangle. The dotted line is the corresponding curve for 2 *CLJ*

$T_B^* = 9\, T_{B,1CLJ}^* = 30.761$. The factor 9 arises because of the 9 site-site interactions. The three curves given are for the parameters $h/l = 0$ (linear 3 *CLJ*), $h/l = 0.433$, and $h/l = 0.866$ (equilateral triangle). For comparison $(T_B^*/T_{B,\text{united atom}}^*)_{2CLJ}$ is also given as a dottted line, from the results of *Kohler* and *Quirke*[1]. In order to visualize the variation with the parameter h/l, Fig. 2 shows $(T_B^*/T_{B,\text{united atom}}^*)_{3CLJ}$ for fixed elongation $L = 0.6$ as function of h/l.

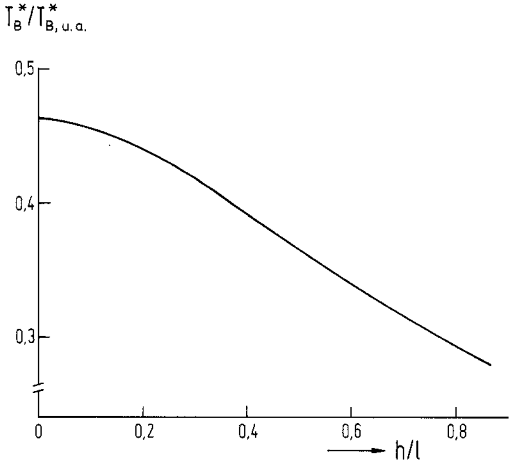

Fig. 2. The reduced *Boyle* temperature of the $3\,CLJ$ at $L = 0.6$, relative to the reduced *Boyle* temperature of the united atom, as function of the relative height of the triangle, h/l

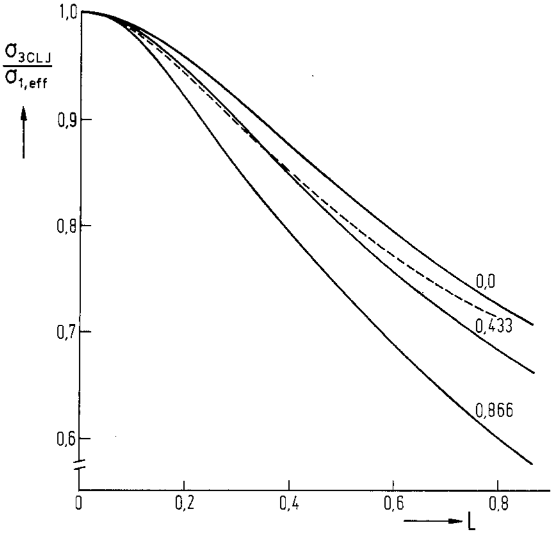

Fig. 3. "Effective" σ-values of $1\,CLJ$-molecules, which produce at $T/T_B = 0.3$ the second virial coefficient of $3\,CLJ$. The notation of the geometry of the $3\,CLJ$ corresponds to Fig. 1. The dotted line is again the corresponding curve for $2\,CLJ$

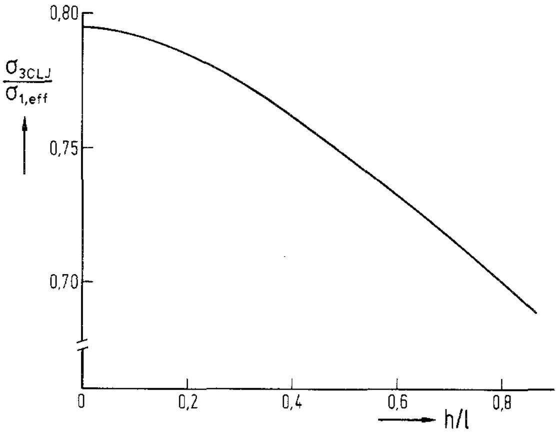

Fig. 4. "Effective" σ-values of 1 *CLJ* at $L = 0.6$ as function of h/l

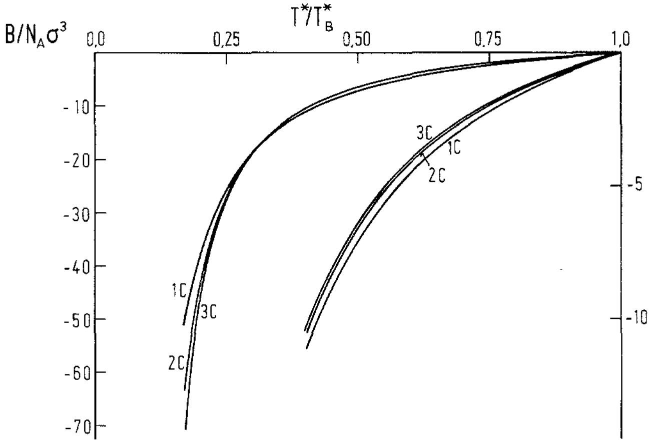

Fig. 5. Reduced second virial coefficients of a 3 *CLJ*-molecule ($L = 0.866$, $h/l = 0.5101$) in comparison to the curves for the equivalent 1 *CLJ* ($\sigma_3/\sigma_{1,\mathrm{eff}} = 0.64633$) and 2 *CLJ* ($L = 0.789$, $\sigma_3/\sigma_{2,\mathrm{eff}} = 0.90537$). The curves for $T > 0.4\ T_B$ are given also on a magnified scale (right ordinate)

Again, following the prescription of *Kohler* and *Quirke* [equ. (6)], it is possible to arrive at "effective" $\sigma_{1,\mathrm{eff}}$-values for 1 *CLJ* molecules, which produce at $T/T_B = 0.3$ exactly the second virial coefficient of the 3 *CLJ* molecule and give a good approximation for $B(T)$ between $T = T_B$ and $T = 0.3\ T_B$. Figs. 3 and 4 show such $\sigma_{3CLJ}/\sigma_{1,\mathrm{eff}}$ ratios for the same states as Figs. 1 and 2. Fig. 5 compares $B(T)$ of a quite anisotropic 3 *CLJ*-molecule, which might serve as model of propane, with that of the equivalent 1 *CLJ*.

It is seen that, indeed, the 1 *CLJ* molecule is a reasonable approximation. A still better approximation should be an equivalent 2 *CLJ* molecule. The question is how to determine the parameter L of the equivalent 2 *CLJ* molecule. One would like to choose L in such a way that also other thermodynamic properties would come out similar. In order to have a simple prescription we suggest to choose L in such a way that the volumes of the corresponding hard molecules are the same. The volume of a hard diatomic can be calculated simply[7], that of a hard triatomic is a more difficult problem, which has been solved by *Rowlinson*[8] and *Powell*[9], and has been treated in a systematic way recently by *Lustig*[10]. The curve for $B(T)$ for the equivalent 2 *CLJ* is also shown in Fig. 5.

Discussion

The similarity of the $B(T)$-curves for 3 *CLJ*-, 1 *CLJ*- and 2 *CLJ*-molecules (with properly defined σ-values) for $T/T_B > 0.3$, where $B(T)$ values can be determined experimentally with good accuracy, makes it difficult to assign molecular shape parameters from second virial coefficients. The situation is quite different at high densities, where, e.g., the properties along the orthobaric curve depend significantly on molecular shape[3,5]. On the other hand, the equivalence conditions established here for 1, 2, and 3 *CLJ* from the point of view of second virial coefficients might help to arrive at a common microscopic scaling of state variables. It is noteworthy, that a linear 3 *CLJ* molecule leads to other scaling conditions than a 2 *CLJ* molecule, as can be readily inferred from Figs. 1 and 3.

Another remark might be of interest. In the theory of fluids, especially mixtures, the idea of group contributions is much discussed. Though this idea is usually applied only to the interaction in excess over the arithmetic mean, we might express it as saying that the interaction energy at contact of a molecule is equal to the sum of interaction energies at contact of its groups. As the interaction energy at contact is about the site-site interaction energy at its minimum, and as this parameter is directly related to the (reduced) *Boyle*-temperature, we can see under which conditions the group interaction idea is valid from the point of view of second virial coefficients. Let us call ε_3 the minimum site-site interaction in a 3 *CLJ*, and let us ask under which condition this is equivalent to $3\,\varepsilon_3 = \varepsilon_1$ of an 1 *CLJ*. As the united atom corresponds to $\varepsilon_3 = \varepsilon_1/9$, our equivalence demands that $(T_B^*/T_{B,\text{united atom}}^*)_{3CLJ} = 1/3$. Looking at Fig. 3, one can see that this is true for $L = 0.52$ for an equilateral triangle, and for $L = 0.87$ for a linear 3 *CLJ* (which corresponds a reduced group-group distance of 0.435). Similarly, for a 2 *CLJ* molecule, the condition would be $(T_B^*/T_{B,\text{united atom}}^*)_{2CLJ} = 1/2$, which holds for $L = 0.49$. Though these L-

values are somewhat smaller than for the most recent models of hydrocarbons ($L = 0.67$ for ethane as $2\,CLJ^{11}$, $L = 0.866$ for propane as $3\,CLJ^{5}$ with a $h/l = 0.5$ ratio intermediate between linear configuration and equilateral triangle, corresponding to a reduced group-group distance of 0.61), one might say that they are roughly met by the carbon groups in organic molecules. But some caution seems to be necessary in applying group contribution ideas to groups with a very different size to elongation ratio.

Table 2. *Reduced second virial coefficients of* 3 *CLJ-molecules as functions of* $T^* = kT/\varepsilon$, $L = l/\sigma$, *and* h/l

$h/l = 0.0$			
L	T_B^*	T^*/T_B^*	$B/(N_A\sigma^3)$
0.05	30.349	0.3	—5.1440
		0.6	—1.2433
		1.05	0.0809
0.10	29.369	0.3	—5.2854
		0.6	—1.2750
		1.05	0.0831
0.20	26.212	0.3	—5.8138
		0.6	—1.3952
		1.05	0.0912
0.27	23.699	0.3	—6.3249
		0.6	—1.5103
		1.05	0.0990
0.3292	21.612	0.3	—6.8474
		0.6	—1.6244
		1.05	0.1061
0.5	16.513	0.3	—8.7645
		0.6	—2.0296
		1.05	0.1312
0.55	15.328	0.3	—9.4213
		0.6	—2.1615
		1.05	0.1408
0.60	14.253	0.3	—10.1452
		0.6	—2.3072
		1.05	0.1474
0.65	13.312	0.3	—10.8905
		0.6	—2.4528
		1.05	0.1576
0.70	12.472	0.3	—11.6781
		0.6	—2.6051
		1.05	0.1662
0.75	11.275	0.3	—12.4871
		0.6	—2.7610
		1.05	0.1759

Table 2 (continued)

$h/l = 0.0$ L	T_B^*	T^*/T_B^*	$B/(N_A\sigma^3)$
0.80	11.056	0.3	—13.3056
		0.6	—2.9180
		1.05	0.1856
0.866	10.269	0.3	—14.4066
		0.6	—3.1209
		1.05	0.2012
0.05	30.303	0.3	—5.1516
		0.6	—1.2451
		1.05	0.0804
0.10	29.240	0.3	—5.3006
		0.6	—1.2772
		1.05	0.0845
0.20	25.720	0.3	—5.8994
		0.6	—1.4154
		1.05	0.0920
0.27	22.952	0.3	—6.4815
		0.6	—1.5463
		1.05	0.1013
0.3292	20.670	0.3	—7.0874
		0.6	—1.6785
		1.05	0.1091
0.50	15.258	0.3	—9.3039
		0.6	—2.1478
		1.05	0.1395
0.55	14.025	0.3	—10.0697
		0.6	—2.3057
		1.05	0.1491
0.60	12.932	0.3	—10.8848
		0.6	—2.4722
		1.05	0.1593
0.65	11.965	0.3	—11.7466
		0.6	—2.6458
		1.05	0.1702
0.70	11.116	0.3	—12.6440
		0.6	—2.8236
		1.05	0.1808
0.75	10.369	0.3	—13.5514
		0.6	—3.0031
		1.05	0.1928
0.793	9.789	0.3	—14.3535
		0.6	—3.161
		1.05	0.2020
0.80	9.699	0.3	—14.4859
		0.6	—3.1865
		1.05	0.2038
0.866	8.193	0.3	—15.7688
		0.6	—3.4324
		1.05	0.2181

$h/l = 0.0$ L	T^*_B	T^*/T^*_B	$B/(N_A\sigma^3)$
0.05	30.303	0.3	—5.1471
		0.6	—1.2429
		1.05	0.0819
0.10	29.121	0.3	—5.3212
		0.6	—1.2832
		1.05	0.0833
0.20	25.413	0.3	—5.9613
		0.6	—1.4268
		1.05	0.0934
0.27	22.472	0.3	—6.5900
		0.6	—1.5709
		1.05	0.1021
0.3292	20.088	0.3	—7.2499
		0.6	—1.7154
		1.05	0.1105
0.5	14.556	0.3	—9.6591
		0.6	—2.2267
		1.05	0.1431
0.55	13.323	0.3	—10.4835
		0.6	—2.3961
		1.05	0.1545
0.60	12.240	0.3	—11.3556
		0.6	—2.5754
		1.05	0.1658
0.65	11.282	0.3	—12.2822
		0.6	—2.7625
		1.05	0.1762
0.70	10.448	0.3	—13.2336
		0.6	—2.9502
		1.05	0.1894
0.75	9.701	0.3	—14.2434
		0.6	—3.1482
		1.05	0.2010
0.80	9.038	0.3	—15.2832
		0.6	—3.3492
		1.05	0.2141
0.866	8.247	0.3	—16.7620
		0.6	—3.6303
		1.05	0.2303
0.05	30.266	0.3	—5.1545
		0.6	—1.2456
		1.05	0.0809
0.10	29.044	0.3	—5.3316
		0.6	—1.2854
		1.05	0.0839
0.20	25.151	0.3	—6.0016
		0.6	—1.4389
		1.05	0.0936

Table 2 (continued)

$h/l = 0.0$ L	T^*_B	T^*/T^*_B	$B/(N_A\sigma^3)$
0.27	22.109	0.3	—6.6751
		0.6	—1.5893
		1.05	0.1033
0.3292	19.666	0.3	—7.3723
		0.6	—1.7417
		1.05	0.1131
0.50	14.065	0.3	—9.9286
		0.6	—2.2840
		1.05	0.1478
0.55	12.837	0.3	—10.8038
		0.6	—2.4645
		1.05	0.1595
0.60	11.758	0.3	—11.7347
		0.6	—2.6565
		1.05	0.1697
0.65	10.823	0.3	—12.6904
		0.6	—2.8472
		1.05	0.1834
0.70	9.990	0.3	—13.7178
		0.6	—3.0505
		1.05	0.1950
0.75	9.251	0.3	—14.7988
		0.6	—3.2608
		1.05	0.2082
0.80	8.591	0.3	—15.9383
		0.6	—3.4784
		1.05	0.2215
0.866	7.813	0.3	—17.5549
		0.6	—3.7813
		1.05	0.2402
0.05	30.239	0.3	—5.1571
		0.6	—1.2460
		1.05	0.0818
0.10	28.910	0.3	—5.3523
		0.6	—1.2909
		1.05	0.0837
0.20	24.777	0.3	—6.0721
		0.6	—1.4547
		1.05	0.0948
0.27	21.580	0.3	—6.8056
		0.6	—1.6182
		1.05	0.1055
0.3292	19.048	0.3	—7.5713
		0.6	—1.7841
		1.05	0.1162
0.5	13.405	0.3	—10.3374
		0.6	—2.3696
		1.05	0.1536

$h/l = 0.0$ L	T_B^*	T^*/T_B^*	$B/(N_A\sigma^3)$
0.55	12.188	0.3	—11.2874
		0.6	—2.5672
		1.05	0.1656
0.60	11.136	0.3	—12.2721
		0.6	—2.7683
		1.05	0.1787
0.65	10.209	0.3	—13.3247
		0.6	—2.9792
		1.05	0.1901
0.70	9.395	0.3	—14.4414
		0.6	—3.1973
		1.05	0.2041
0.75	8.669	0.3	—15.6421
		0.6	—3.4261
		1.05	0.2185
0.80	8.016	0.3	—16.9515
		0.6	—3.6731
		1.05	0.2321
0.866	7.249	0.17	—70.8849
		0.2	—46.2496
		0.3	—18.8530
		0.4	—10.4187
		0.5	—6.3765
		0.6	—4.0210
		0.7	—2.4852
		0.8	—1.4042
		0.9	—0.6109
		1.05	0.2536
0.05	30.157	0.3	—5.1679
		0.6	—1.2484
		1.05	0.0817
0.10	28.612	0.3	—5.3945
		0.6	—1.3003
		1.05	0.0844
0.20	23.878	0.3	—6.2554
		0.6	—1.4959
		1.05	0.0969
0.27	20.392	0.3	—7.1275
		0.6	—1.6893
		1.05	0.1098
0.3292	17.721	0.3	—8.041
		0.6	—1.8881
		1.05	0.1221
0.50	12.107	0.3	—11.2933
		0.6	—2.5723
		1.05	0.1658
0.55	10.943	0.3	—12.3893
		0.6	—2.7980
		1.05	0.1796

Table 2 (continued)

$h/l = 0.0$			
L	T_B^*	T^*/T_B^*	$B/(N_A\sigma^3)$
0.60	9.950	0.3	—13.5322
		0.6	—3.0327
		1.05	0.1946
0.65	9.046	0.3	—14.8382
		0.6	—3.2775
		1.05	0.2093
0.70	8.261	0.3	—16.2619
		0.6	—3.5472
		1.05	0.2256
0.75	7.570	0.3	—17.8389
		0.6	—3.8387
		1.05	0.2438
0.80	6.961	0.3	—19.5738
		0.6	—4.1540
		1.05	0.2621
0.866	6.272	0.3	—22.0863
		0.6	—4.6018
		1.05	0.2880
0.05	30.030	0.3	—5.1837
		0.6	—1.2515
		1.05	0.0826
0.10	28.129	0.3	—5.4655
		0.6	—1.3160
		1.05	0.0861
0.20	22.599	0.3	—6.5449
		0.6	—1.5612
		1.05	0.1009
0.27	18.815	0.3	—7.6321
		0.6	—1.7983
		1.05	0.1172
0.3292	16.077	0.3	—8.7578
		0.6	—2.0423
		1.05	0.1327
0.50	10.653	0.3	—12.6553
		0.6	—2.8488
		1.05	0.1841
0.55	9.543	0.3	—14.0745
		0.6	—3.1267
		1.05	0.2005
0.60	8.591	0.3	—15.6220
		0.6	—3.4248
		1.05	0.2182
0.65	7.770	0.3	—17.3395
		0.6	—3.7462
		1.05	0.2390
0.70	7.060	0.3	—19.2603
		0.6	—4.0993
		1.05	0.2583

$h/l = 0.0$ L	T_B^*	T^*/T_B^*	$B/(N_A\sigma^3)$
0.75	6.456	0.3	—21.2907
		0.6	—4.4650
		1.05	0.2813
0.80	5.934	0.3	—23.4966
		0.6	—4.8482
		1.05	0.3039
0.866	5.352	0.3	—26.6979
		0.6	—5.3910
		1.05	0.3354

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