STRUCTURE OF HARD BODY FLUIDS. A CRITICAL COMPILATION OF SELECTED COMPUTER SIMULATION DATA

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Computer simulation data on structural properties [spherical harmonic expansion coefficients of the full pair correlation function $g(1, 2)$, radial slices through $g(1, 2)$, the background correlation function $y(1, 2)$ and the triplet correlation function (for hard spheres), various angle averages of $g(1, 2)$ and, for hard spheres, also the direct correlation and bridge functions] of pure hard body fluids known to date have been critically assessed and tables of selected data are presented. In addition to the tables, parametrizations of the data are also given whenever they have been available. The molecular models considered include both convex body models (spheres and prolate spherocylinders) and interaction-site models (homo- and heteronuclear diatomics, linear and nonlinear symmetric triatomics, and tetrahedral penta-atomics).

1. INTRODUCTION

Computer simulations provide, strictly speaking, the only experimental means of the statistical thermodynamics of liquids and have played thus a key role in its development: only the simulations made it possible to reveal links between the bulk properties and intermolecular forces. A typical example is the finding that the structure of normal fluids (i.e. fluids without strong long-ranged forces and H-bonds) is determined primarily by strong short-ranged repulsive forces. This finding gave then rise to nowadays widely used perturbation theories employing a hard body reference. Besides this practical importance, hard body fluids also serve as simplest models of molecular fluids on which various ideas, approaches, and theories are tested. For these reasons as best as possible knowledge of hard body fluid properties is required.

A number of review papers and monographs has been devoted to computer simula-

tions (see e.g. refs[43,55,56,60]) but they all focus primarily on the method itself and its realization. The only exception seem two review papers by Levesque et al.[31]. They contain nearly exhausting bibliography on simulations on fluids up to 1983 and data on various bulk properties. However, structural data are discussed only in connection with theoretical predictions and no tablets thereof are provided.

When dealing with presentation of simulation results one has to distinguish between the thermodynamic and structural data. Because of their dependence only on density (for hard body fluids) and on parameters defining the model, thermodynamic data are easily presented in tables. Structural properties however depend, in addition to the above variables, also on the positions and orientations of particles which makes their presentation too space exacting. For this reason authors of structural simulation data often refer to them as to unpublished results or show only some selected results on graphs. Also very often the simulations are not the primary aim of the research but their output is further used, for instance, for evaluating macroscopic properties. As a result, information essential to many theorists remains again unavailable. With rapidly developing computer technology there is nowadays no problem for anybody to run a computer and obtain within a few hours pseudo-experimental data on a studied system for the required set of state variables in order to make checks and comparisons. Such data are, however, usually only one-purpose and make later quantitative comparison of different theories difficult or even impossible. Further, to account for all tiny effects influencing the results and to produce simulation data of top accuracy is the time consuming and quite unpopular task (in fact, the same applies to classical laboratory experiments, too). For all these reasons it seems very useful to have certain generally available standards and this has been the motivation for this review.

The paper is organized as follows. In the following section there are given the definitions of all considered functions and basic relationships. Separate sections are then devoted to the fluid of hard spheres (Section 3), convex body fluids (Section 4), and fluids made up of fused-hard-sphere particles (Section 5). In these sections the available data are shortly assessed and details on the data listed in tables, which take up the rest of the paper, are given. It has not been the intention of this review to provide, besides the data themselves, also an exhausting bibliography on simulations on hard body fluids performed to date. Only those data are therefore mentioned which we considered relevant. On the other hand, it may have happened that some important data have completely slipped away from our attention. In such a case we would appreciate very much being notified on such data.

In addition to our own computer simulation data, we also have been collecting for years data produced by other authors and we are grateful to all who made their unpublished data available to us. Particularly, we want to record our thanks to R. D. Groot, R. I. M. Laboratory, Nijmegen, M. Rigby, King's College, London, and W. B. Streett, Cornell University, Ithaca, whose data appear in this review.

2. BASIC DEFINITIONS AND RELATIONSHIPS

Let us consider a homogeneous fluid made up of N particles confined to a volume V at a temperature T. Position of particle i is defined by the radius vector $\boldsymbol{R}_i$ of an arbitrary chosen reference point within the particle and by its orientation $\boldsymbol{\Omega}_i$.

For a hard particle fluid the total potential energy U, $U = U(1, \ldots, N) \equiv \equiv U(\boldsymbol{R}_1, \boldsymbol{\Omega}_1, \ldots, \boldsymbol{R}_N, \boldsymbol{\Omega}_N)$ is pair-wise additive, $U = \sum_{i,j} u(i, j)$, where the pair potential u takes on two values only regardless of the model considered:

$$u(i, j) \equiv u(\boldsymbol{R}_i, \boldsymbol{\Omega}_i, \boldsymbol{R}_j, \boldsymbol{\Omega}_j) = \begin{cases} +\infty & \text{if particles } i \text{ and } j \text{ overlap} \\ 0 & \text{otherwise .} \end{cases} \qquad (1)$$

Hard bodies model in the simplest way the steep repulsive forces between real molecules at short separations and should thus copy, at least approximately, their size and shape. The core of a spherically symmetric molecule (e.g. argon) is evidently modelled by a sphere. For polyatomic molecules there are, in principle, two possibilities how to describe their shape: by a fused-hard-sphere (FHS) model or by a convex body (CB) model.

The FHS model views molecules as a set of interaction sites each being represented by a hard sphere (hs) of diameter σ_α. Hence,

$$u(1, 2) = \sum_{\alpha,\beta} u_{\mathrm{hs}}(r_{\alpha\beta}) , \qquad (2)$$

where $r_{\alpha\beta} \equiv r_{\alpha\beta}(\boldsymbol{R}_1, \boldsymbol{\Omega}_1, \boldsymbol{R}_2, \boldsymbol{\Omega}_2)$ is the distance between site α on particle 1 and site β on particle 2. The FHS models investigated to date are depicted in Fig. 1. These are homonuclear and heteronuclear diatomics (dumbbells), linear and nonlinear symmetric triatomics and tetrahedral pentaatomics.

The other group of models, the CB models, mimicks the entire molecule or its core by a convex body and a measure of the particle separation in this case is the shortest surface-to-surface distance s (for details of the CB geometry see e.g. Kiha-

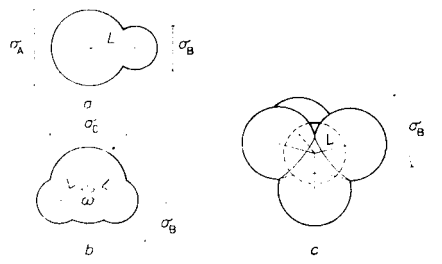

FIG. 1

Fused-hard-sphere models of general diatomic (*a*), symmetric triatomic (*b*), and tetrahedral pentaatomic (*c*) molecules

ra[20]). Variety of up to date considered CB models is somewhat larger in comparison with the FHS models, but overwhelming majority of computations has aimed only at obtaining data on virial coefficients and the equation of state (for a review see ref.[8]). We are thus aware of data on structure only for prolate and oblate spherocylinders. These two models are depicted in Fig. 2.

The structure of a fluid is described, in general, by a set of correlation functions (c.f.) g_h defined (in the canonical ensemble) as follows:

$$g_h(1, \ldots, h) = \frac{N!}{(N-h)!}\left(\frac{V}{N}\right)^h \int \ldots \int \exp\left[-\beta U\right] \mathrm{d}(h+1) \ldots \mathrm{d}(N) \Big/ \int \ldots \int \exp\left[-\beta U\right] \mathrm{d}(1) \ldots \mathrm{d}(N) \,. \tag{3}$$

Here $\beta = 1/\boldsymbol{kT}$, $\boldsymbol{k}$ is the Boltzmann constant and T absolute temperature, and $\mathrm{d}(i)$ stands for differentials $\mathrm{d}\boldsymbol{R}_i\,\mathrm{d}\boldsymbol{\Omega}_i$, $\int \mathrm{d}\boldsymbol{\Omega}_i = 1$. Denoting by n the number density, $n = N/V$, then the function $n^h g_h$ gives the probability density of finding h molecules in volume elements $\mathrm{d}(1), \ldots, \mathrm{d}(h)$ around $(\boldsymbol{R}_1, \boldsymbol{\Omega}_1), \ldots, (\boldsymbol{R}_h, \boldsymbol{\Omega}_h)$ regardless of positions and orientations of the remaining molecules. The first function of the set equals unity,

$$g_1(1) = 1 \,, \tag{4}$$

and expresses the fact that the probability of finding a molecule at any point within the volume V is constant in the homogeneous fluid.

The most important of all correlation functions is the pair correlation function (p.c.f.) g_2: for systems with pair-wise additive interactions it provides the necessary information required for evaluating thermodynamic properties. With the exception of the hard sphere fluid we confine our considerations in this paper only to this correlation function and drop subscript 2 in the following text.

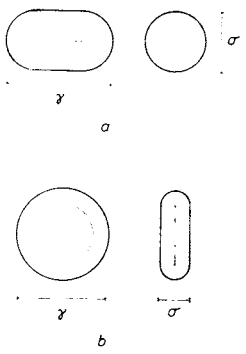

FIG. 2

Convex body models of prolate (*a*) and oblate (*b*) spherocylinders

Higher order c.f. are rarely studied and, moreover, only for spherically symmetric potentials. A certain attention has been paid to g_3 of hard spheres in connection with integrodifferential equations and higher-order corrections to perturbation expansions (for details see e.g. Hansen and McDonald[18]). Functions g_4 and higher seem completely "terra incognita" at present.

While the pair potential and potential-related functions of hard bodies are discontinuous, the background c.f. y, called also the cavity distribution or simply y-function by some authors,

$$y(1, 2) = g(1, 2) \exp [\beta u(1, 2)] , \tag{5}$$

remains continuous at the points of discontinuity of the potential. This function can be interpreted as the correlation function of two cavities (i.e. a pair of molecules which interact with other molecules in the usual way but which do not interact between themselves; it means, they can overlap). This interpretation makes it possible to devise a special algorithm for its evaluation from simulations[2,25,40].

The next two structural functions are not the primary outputs from simulations but can be obtained for spherical particles by a careful analysis of the p.c.f. The first one, the direct correlation function (d.c.f.) c, is defined by the Ornstein–Zernike (O–Z) equation,

$$h(1, 2) = c(1, 2) + n \int c(1, 3)\, h(2, 3)\, \mathrm{d}(3) , \tag{6}$$

where $h = g - 1$ is the total correlation function. The other function is the bridge function, $B(1, 2)$, which is given by an infinite sum of elementary diagrams,

$$B(1, 2) = h(1, 2) - c(1, 2) - \ln [y(1, 2)] . \tag{7}$$

The functions c and B are known only for the hard sphere fluid and details of their evaluation are described in Section 3.

The complete description of the p.c.f. for a non-spherical molecule fluid is an extremally complicated task. The p.c.f. is, at a given density, a function of at least four variables (distance and mutual orientation of a pair of molecules) and it is therefore practically impossible to evaluate it from simulations. There are three ways which have been used to characterize the structure of molecular fluids. The most frequently used method is the expansion of g (and, similarly, any other function depending on separation R, $R = |\boldsymbol{R}_1 - \boldsymbol{R}_2|$, and orientations) using spherical harmonics[48]. In the second method radial slices, i.e. values for a specific set of angular variables, are evaluated. Finally, in the third method the structure is described by means of constrained unweighted angular averages of $g(1, 2)$; a typical example of such a function is the average site–site pair correlation function, $G_{\alpha\beta}$. It must be however reminded that both the slices and functions $G_{\alpha\beta}$ provide only

partial information on the system, although an attempt was made[42] to reconstruct the full $g(1, 2)$ from $G_{\alpha\beta}$ but without greater success.

When expanding g by means of the spherical harmonics, $g(1, 2)$ is defined by an (infinite) set of the spherical harmonic expansion coefficients. There are two alternative forms of the spherical harmonic expansion. The first, a more general form, employes a space-fixed coordinate frame and is mainly used in theoretical calculations. The other form, which is a simplification of the former one, uses the intermolecular frame defined by the vector formed by the reference points of the molecules, see Fig. 3.

With respect to mathematical simplicity and majority of existing data we confine here our considerations to linear molecules and the intermolecular frame. The p.c.f. at a given separation R and orientations $\boldsymbol{\Omega}_i = (\vartheta_i, \phi_i)$ is then given by

$$g(R, \boldsymbol{\Omega}_1, \boldsymbol{\Omega}_2) = 4\pi \sum_{k=0}^{\infty} \sum_{l=0}^{\infty} \sum_{m=|k-l|}^{k+l} g_{klm}(R)\, Y_{km}(\boldsymbol{\Omega}_1)\, Y_{l\bar{m}}(\boldsymbol{\Omega}_2)\,, \tag{8}$$

where $\bar{m} = -m$ and $Y_{km}(\boldsymbol{\Omega})$ is the spherical harmonics. Values of the spherical harmonic expansion coefficients $g_{klm}(R)$ are calculated directly in computer simulations using

$$g_{klm}(R) = 4\pi \langle g(R, \boldsymbol{\Omega}_1, \boldsymbol{\Omega}_2)\, Y^*_{km}(\boldsymbol{\Omega}_1)\, Y^*_{l\bar{m}}(\boldsymbol{\Omega}_2) \rangle\,, \tag{9}$$

where the asterisk denotes conjugate values and $\langle \ldots \rangle$ denotes an unweighted average over orientations. In the case of nonlinear bodies the relative orientation of a pair of a particles depends, in addition to ϑ_1, ϑ_2, and ϕ, also on twisting angles Λ_1 and Λ_2. A generalized spherical harmonic expansion coefficient, Γ_{klm}, may be defined analogously to Eq. (9), where now the p.c.f. is a function of all five angular variables and $\langle \ldots \rangle$ means an unweighted average over all orientations (for details see Labík and Nezbeda[27]). For hard body systems the spherical harmonic expansion coefficients, with the exception of the leading 000-term, are generally significant only at shorter interparticle separations. With increasing separation they rapidly decay and are virtually zero beyond, approximatelly, double the particle's size. At larger separations they thus indicate the scatter of data and point indirectly to their accuracy.

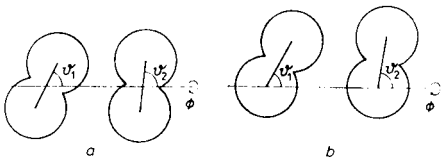

FIG. 3
Definition of the intermolecular CC (*a*) and SS (*b*) frames

When the molecules are symmetric (e.g. spherocylinders or homonuclear diatomics), the centre of the symmetry of molecule is probably the most natural choice for the reference point. With this choice (called the centre–centre or CC frame) symmetry considerations considerably reduce the number of harmonic coefficients contributing to sum (*8*). For instance, for linear symmetric particles the only non-vanishing coefficients are those with even indices k and l. When the reference point coincides with an interaction site (e.g. with the centre of either sphere for diatomics) we shall refer to this choice as the SS (site–site) frame and use capital letters for the corresponding quantities, e.g. G_{klm} or, more specifically, $G^{\alpha\beta}_{klm}$, in order to distinguish them from those in the CC frame.

For calculating radial slices one can, in principle, choose any specific set of fixed values of variables but those actually used correspond to the parallel, crossed, T-shaped, and end-to-end configurations (see Fig. 4). Computer data on these slices can serve as a stringent test of the spherical harmonic expansion and/or accuracy of theory. However, evaluation of the slices from simulations is not a trivial matter. An enourmous number of configurations must be generated in order to obtain a reasonable result and this is the reason why the slices through $g(1, 2)$ are known only for homonuclear diatomics and prolate spherocylinders, and through $y(1, 2)$ only for homonuclear diatomics.

The average site-site c.f. $G_{\alpha\beta}$ (denoted sometimes also as G_{ss}) for a fluid of FHS particles is defined as follows:

$$G_{\alpha\beta}(r) = \int_{r=\text{const}} g(1, 2)\, \mathrm{d}(1)\, \mathrm{d}(2)\,. \qquad (10)$$

It is proportional to the probability density of finding site α of particle 1 at a distance $r \equiv r_{\alpha\beta}$ apart from site β of particle 2 regardless of positions of the remaining sites of particles 1 and 2 and of positions and orientations of all the remaining particles of the system. Functions $G_{\alpha\beta}$ possess a distinctive property, the so called cusps

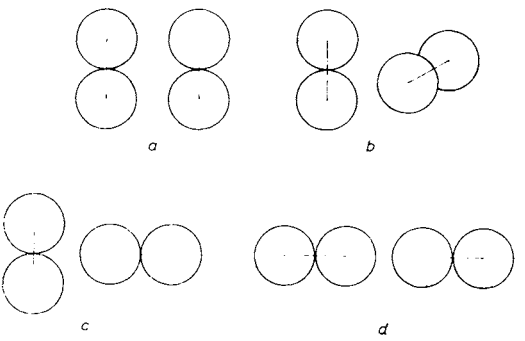

FIG. 4
Definition of parallel ((*a*); $\vartheta_1 = \vartheta_2 = \pi/2$, $\phi = 0$), crossed ((*b*); $\vartheta_1 = \vartheta_2 = \phi = \pi/2$), T-shaped ((c); $\vartheta_1 = \pi/2$, $\vartheta_2 = 0$), and end-to-end ((*d*); $\vartheta_1 = \vartheta_2 = 0$) configurations

(discontinuities in the first derivative) at characteristic separations. (We remind in passing that for the fluid of hard spheres such a discontinuity does not appear in the first but in the second derivative). These cusps are a simple consequence of the exact cluster expansion but they can also be explained simply in terms of molecular geometry (see e.g. a detailed discussion concerning the cusps for a hard heteronuclear diatomic fluid in ref.[51]). When $g(1, 2)$ is expressed with respect to the α–β SS frame, then $G_{\alpha\beta}$ coincides with the leading spherical harmonic expansion coefficient, $G_{\alpha\beta} \equiv \equiv G^{\alpha\beta}_{000}$. The average site–site c.f. $G_{\alpha\beta}$ are of great interest because their analogues for real fluids can be obtained from scattering experiments and for hard body fluids they are readily obtainable with reasonable accuracy from the RISM theory[10]. Also the spherical harmonic expansion coefficients $G^{\alpha\beta}_{100}$ are of great importance because they are required for the evaluation of the equation of state[27].

For CB models a counterpart of the average site–site correlation function is the surface-to-surface correlation function $g_s(s)$,

$$g_s(s) = \int_{s=\text{const}} g(1, 2)\, \mathrm{d}(1)\, \mathrm{d}(2)\,, \tag{11}$$

where s denotes the shortest surface-to-surface distance at a given separation R and orientations $\boldsymbol{\Omega}_1$ and $\boldsymbol{\Omega}_2$.

The crucial point of the data selection is assessment of their accuracy and reliability. From the two general simulation methods, Monte Carlo (MC) and molecular dynamics (MD), the latter is only rarely used for nonspherical hard body fluids (an exception is an approximate MD method developed by Chapela and co-workers[12]), and we confine therefore our discussion to the MC method only. A typical MC experiment is characterized primarily by the number of particles, N, the total number of equilibrium configurations generated, N_c, the number of configurations used in the analysis to obtain the observables of interest, N_a, and by the acceptance ratio. Small number of particles causes, roughly, the systematic error of the order of $1/N$ and it also defines (in dependence on density) the maximum interparticle distance R_m up to which a structural quantity can be determined. The acceptance and N_a/N_c ratios influence directly the accuracy of results and effectiveness of the experiment. For N_a/N_c close to unity smoother results are obtained but this does not necessarily means that, due to strong correlations between subsequent configurations, the results are more accurate. The role of the acceptance ratio was discussed by Streett and Gubbins[50] but their conclusions were rather vague. In majority of simulations the ratio was kept at the 50 per cent level or slightly lower. In a recent theoretical paper[22] on effectiveness of the MC simulations it has been shown that the optimum ratio may be as low as 10 per cent. An ineffective sampling of the configuration space may, however, be compensated by considerable extending the chain of generated configurations. Until recently the error of the experiment has been always determined in the same way: the whole experiment is devided into subruns which are sup-

posed to be statistically independent and the standard methods are then used. Only recently several papers[5,21,45,46,49] have appeared dealing more rigorously with estimation of the errors making use of the autocorrelation coefficients.

It is obvious that the amount of data available decreases with increasing complexity of models. For spheres and homonuclear diatomics, for instance, we can thus select the data of the top acuracy, while for some systems only one set of data is available. It cannot be said that all authors bother about reporting technical details of their simulations nor they pay a proper attention to error estimation. In addition to the information which can be extracted directly from the published papers, we thus have performed in some cases additional consistency checks in order to better assess the data.

As a consequence of Eq. (*1*), properties of the hard body fluids depend, in the N–V–T ensemble, only on one thermodynamic parameter: the number density n, $n = N/V$. Three different definitions of a dimensionless density can be found in literature: (i) $n^* = n\sigma^3$, (ii) $\eta = nV_m$, and (iii) $\bar{n} = nd^3$. In choice (i) σ means a characteristic size of a particle, for instance the diameter of either sphere for diatomics. η is the so called packing fraction and V_m stands for the volume of a particle. In choice (iii) d denotes the diameter of a sphere of the same volume, $d^3 = 6V_m/\pi$. There are several reasons why to prefer the packing fraction, but we will also use in this paper the reduced density n^*.

Throughout the paper we label the larger sphere of diatomics as A and the central sphere of polyatomics as C; other sites of both diatomics and polyatomics are labelled as B. Further, for simplicity, diameters of spheres A and C, respectively, are used as a length unit for FHS models; for spherocylinders all the distances are scaled by their breadth.

3. HARD SPHERES

The fluid made up of hard spheres is the simplest and most intensively studied system. Simulated results are known for g_2, g_3, and y. In addition to these, the direct c.f. and the bridge function have been extracted from the simulation data and all these functions but g_3 have been also parametrized.

The first simulation providing the p.c.f. goes back to fifties[44] and since a number of simulations has been performed (for a review on early simulations up to 1967 see Wood[60] and for simulations up to 1983 see Levesque et al.[31]). For a long time the most frequently quoted and used data have been those of Barker and Henderson[3,4]. These data ($N = 108$, $R_m = 2{\cdot}27$, $N_c = 10^6$) cover the range of densities n^* ranging from 0·2 to 0·925. Accuracy of the data was not given, but comparing them with newer results we estimate their accuracy to be within 0·01 – 0·02 with slightly larger uncertainty near the contact at high densities.

The hard sphere fluid has been recently carefully reexamined[14,16,23,24,26] using larger numbers of particles, configurations, and more sophisticated methods to sample the configuration space. Very accurate simulations by Erpenbeck and Wood[14] (a combination of MC and MD methods) focus on the equation of state only, and so the best data on the p.c.f. for densities up to $n^* = 0{\cdot}9$ seem those by Groot et al.[16] (N depends on density and varies from 549 for $n^* = 0{\cdot}2$ to 2 470 for $n^* = 0{\cdot}9$; $R_m = 7$, $N_c = 5 \cdot 10^7$) which are complemented for $n^* = 0{\cdot}925$ and 0·94 (densities close to the phase transition) by a new data by Labík and Malijevský[26] $N = 256$, $R_m = 3$, $N_c = 5 \cdot 10^6$). Both these recommended data are given in Table I (Groot et al. did not publish tables of g; values in this table are smoothed data of their raw computer outputs).

The triplet c.f. g_3 is a function of three variables, $g_3 \equiv g_3(R_{12}, R_{13}, R_{23})$,and its complete determination is practically impossible. g_3 is therefore characterized by its values at specific triplet geometries (two choices are used: (i) triplets for which one of the sides falls within the range $R_i \pm \delta$, and (ii) isosceles and equilateral configurations), although an attempt has recently been made[17] to express g_3 also by means of the spherical harmonic expansion. Despite its importance in integrodifferential equations[18], we were aware of only two data sets on g_3: one set due to Alder[1] which gives only a few values of g_3 at limited geometries (choice (ii)) and at solid and very high density fluid regions and the other newer set by Uehara et al.[54] who employ choice (i) for triplet geometries. When the manuscript of this review was nearly ready, we came across the third set due to McNeil et al.[34]. These data (choice (ii) for geometries) have been deposited with the AIP's Physics Auxiliary Publication Service (document No. PAPS JCPSA-78-388-39) and for this reason we show in Table II only the data due to Uehara et al. ($N = 108$ and 256, $N_c = 2{\cdot}3 \cdot 10^6$). In this table there is not directly given g_3 but the ratio $g_3/g_2(R_{12}) \cdot g_2(R_{13})\, g_2(R_{23})$ because it varies more smoothly than g_3 itself. Uehara et al. also give in their Table II the p.c.f. at even values of $10.R_{12}$; at odd values we have completed the table by adding the p.c.f. obtained from the O–Z equation and Eq. (*16*) for the bridge function. The p.c.f. obtained in this way is indistinguishable from the MC values.

The background c.f. was simulated by Patey and Torrie[40] (MC with the umbrella sampling, $N = 108$ and 864, $N_c = 2 \cdot 10^7$) at $n^* = 0{\cdot}8$. Error of the data as estimated by the authors is relatively large: between 10 and 20 per cent at $R < 0{\cdot}63$ and between 5 and 10 per cent at larger separations. Labík and Malijevský[25] developed a technique of simulating y which complements, in a certain sense, the umbrella sampling. The method is very efficient at low and medium densities and also at small separations. The function y was obtained at $n^* = 0{\cdot}3$, 0·5, and 0·7 ($N = 256$; $N_c = 10^5$, 10^6, and $2 \cdot 10^6$ for $n^* = 0{\cdot}3$, 0·5 and 0·7, respectively) with the standard deviation of the order of 0·1 per cent at small separations. The error increases with increasing separation and is about a few per cent at contact. Somewhat later Ballance and

TABLE I
The fluid of hard spheres: pair correlation function g(R)

	η					
R	0.20944	0.31416	0.41888	0.47124	0.48433	0.49218
1.000	1.816	2.622	4.039	5.175	5.527	5.755
1.025	1.753	2.422	3.488	4.271	4.499	4.650
1.050	1.687	2.246	3.042	3.539	3.683	3.765
1.075	1.623	2.086	2.668	2.955	3.051	3.090
1.100	1.561	1.947	2.347	2.493	2.540	2.550
1.125	1.506	1.815	2.075	2.125	2.141	2.128
1.150	1.458	1.704	1.854	1.829	1.825	1.808
1.175	1.414	1.600	1.664	1.587	1.567	1.541
1.200	1.370	1.504	1.502	1.390	1.363	1.334
1.225	1.330	1.424	1.360	1.229	1.198	1.164
1.250	1.290	1.351	1.241	1.099	1.062	1.031
1.275	1.254	1.283	1.139	0.992	0.950	0.924
1.300	1.221	1.220	1.056	0.905	0.863	0.833
1.325	1.188	1.161	0.982	0.832	0.793	0.764
1.350	1.158	1.110	0.919	0.772	0.735	0.706
1.375	1.130	1.064	0.868	0.725	0.686	0.663
1.400	1.107	1.024	0.826	0.689	0.651	0.628
1.425	1.088	0.990	0.792	0.659	0.623	0.602
1.450	1.067	0.962	0.764	0.638	0.602	0.586
1.475	1.046	0.937	0.741	0.624	0.592	0.575
1.500	1.028	0.917	0.723	0.616	0.589	0.574
1.525	1.012	0.897	0.711	0.615	0.587	0.578
1.550	0.996	0.881	0.706	0.620	0.596	0.584
1.575	0.983	0.867	0.707	0.630	0.611	0.602
1.600	0.971	0.856	0.709	0.646	0.632	0.626
1.625	0.962	0.849	0.717	0.668	0.660	0.657
1.650	0.953	0.845	0.729	0.697	0.696	0.697
1.675	0.946	0.842	0.747	0.732	0.738	0.741
1.700	0.941	0.845	0.771	0.775	0.789	0.796
1.725	0.939	0.851	0.799	0.824	0.842	0.856
1.750	0.935	0.857	0.827	0.876	0.902	0.919
1.775	0.933	0.864	0.859	0.930	0.969	0.988
1.800	0.934	0.874	0.895	0.984	1.030	1.053
1.825	0.934	0.887	0.934	1.036	1.082	1.108
1.850	0.937	0.901	0.973	1.083	1.129	1.154
1.875	0.940	0.917	1.008	1.124	1.170	1.192

TABLE I
(Continued)

R	η					
	0.20944	0.31416	0.41888	0.47124	0.48433	0.49218
1.900	0.945	0.936	1.044	1.159	1.197	1.220
1.950	0.959	0.978	1.116	1.222	1.253	1.268
1.975	0.967	1.000	1.151	1.253	1.279	1.296
2.000	0.976	1.022	1.185	1.289	1.320	1.329
2.025	0.987	1.044	1.211	1.310	1.335	1.347
2.050	0.994	1.060	1.221	1.304	1.324	1.333
2.075	0.998	1.070	1.216	1.279	1.293	1.296
2.100	1.004	1.076	1.201	1.241	1.248	1.246
2.125	1.007	1.078	1.181	1.198	1.200	1.194
2.150	1.012	1.078	1.158	1.152	1.148	1.136
2.175	1.015	1.077	1.131	1.107	1.099	1.083
2.200	1.016	1.073	1.103	1.064	1.050	1.033
2.225	1.019	1.068	1.074	1.023	1.005	0.988
2.250	1.017	1.062	1.047	0.987	0.966	0.947
2.275	1.018	1.055	1.022	0.954	0.929	0.913
2.300	1.018	1.048	1.000	0.924	0.901	0.882
2.325	1.019	1.042	0.981	0.901	0.872	0.858
2.350	1.018	1.034	0.963	0.881	0.855	0.840
2.375	1.018	1.026	0.948	0.866	0.841	0.825
2.400	1.016	1.017	0.934	0.856	0.832	0.817
2.425	1.012	1.009	0.922	0.850	0.830	0.814
2.450	1.011	1.001	0.915	0.848	0.828	0.816
2.475	1.009	0.996	0.911	0.850	0.831	0.823
2.500	1.009	0.992	0.909	0.854	0.839	0.835
2.550	1.008	0.984	0.911	0.874	0.869	0.871
2.600	1.004	0.979	0.919	0.906	0.912	0.919
2.650	1.002	0.975	0.935	0.947	0.960	0.974
2.700	0.999	0.973	0.956	0.991	1.017	1.027
2.750	0.997	0.976	0.980	1.031	1.062	1.076
2.800	0.997	0.979	1.004	1.064	1.095	1.111
2.850	0.997	0.983	1.026	1.086	1.114	1.126
2.900	0.997	0.990	1.041	1.094	1.118	1.126
2.950	0.996	0.997	1.051	1.092	1.108	1.110
3.000	0.997	1.004	1.056	1.082	1.089	1.089

Speedy[2] reported results for y at several densities but their data are only of fair accuracy. The direct simulation data by Labík and Malijevský are listed in Table III. In this table there are also shown the data by Patey and Torrie evaluated from a polynomial of the third degree fitted to their original data (maximum deviation of the fit from the data is only a few per cent, i.e. much less than the estimated accuracy). The reason for this fitting was to show both data at the same separations.

The direct c.f. is not directly measurable in simulations but can be obtained from the O–Z relation using data on the p.c.f. The usual way is to use the Fourier transform but this way is known to be numerically unstable and requires the p.c.f. of very high accuracy. Such calculations were performed by Groot et al.[16] who used their own data of g and obtained c for densities n^* ranging from 0·2 to 0·9 and for separations from 0 to 2. Parametrization of these data reads as follows:

$$c(R) = (c_0 + c_1 R + c_2 R^2 + c_3 R^6)(1 - \eta)^{-4}, \quad R < 1, \tag{12}$$

where

$$\begin{aligned} c_0 &= -1 - 4{\cdot}084239\eta - 4{\cdot}207343\eta^2 + 3{\cdot}616491\eta^3 \\ c_1 &= 5{\cdot}694732\eta + 11{\cdot}910265\eta^2 - 8{\cdot}567493\eta^3 \\ c_2 &= 0{\cdot}375078\eta - 9{\cdot}793214\eta^2 + 8{\cdot}155003\eta^3 \\ c_3 &= -0{\cdot}485572\eta + 2{\cdot}590295\eta^2 - 4{\cdot}537336\eta^3 \end{aligned} \tag{13}$$

TABLE II
The fluid of hard spheres: background correlation function y(R). (Numbers in parentheses denote the error of last digits)

	η			
R	0.15708	0.26180	0.36652	0.41888
0.00	5.748	45.42	1604.0	23900.(3000)
0.10	4.973(12)	32.340(36)	789.9(25)	8800.(1000)
0.20	4.319(11)	23.080(21)	390.0(19)	3240.(600)
0.30	3.739(10)	16.490(34)	194.9(14)	1200.(200)
0.40	3.244(5)	11.850(34)	97.90(97)	454.(60)
0.50	2.820(6)	8.588(25)	50.40(84)	177.(30)
0.60	2.469(3)	6.306(18)	26.60(62)	72.(15)
0.70	2.166(4)	4.697(22)	14.70(44)	31.(2)
0.80	1.921(5)	3.559(17)	8.37(39)	14.4(10)
0.90	1.713(5)	2.736(12)	5.00(26)	7.2(5)
1.00	1.541(9)	2.150(12)	3.09(16)	3.9(3)

TABLE III

The fluid of hard spheres: slices through the triplet correlation function $g_3(R_{12},R_{13},R_{23})$ at the contact of spheres 2 and 3 ($R_{23}=1$)

		R_{13}					
R_{12}	$g_2(R_{12})$	1.0	1.1	1.2	1.6	2.0	2.2
				η = 0.2207			
1.00	1.906	0.790	0.802	0.829	0.997	1.035	
1.10	1.601	0.802	0.847	0.825	1.003	1.027	
1.20	1.390	0.829	0.825	0.887	1.016	1.029	0.974
1.30	1.225	0.876	0.921	0.947	1.018	1.029	0.977
1.40	1.107	0.931	0.943	0.948	1.020	1.025	0.975
1.50	1.019	0.947	0.981	0.951	1.021	1.012	0.995
1.60	0.967	0.997	1.003	1.016	1.032	1.027	0.980
1.70	0.931	1.046	1.022	1.048	1.026	1.009	0.992
1.80	0.920	1.092	1.097	1.051	1.020	1.015	0.957
1.90	0.941	1.048	1.097	1.052	1.033	0.988	0.984
2.00	0.978	1.035	1.027	1.029	1.027	1.003	0.989
2.10	1.008		0.991	0.996	0.985	0.981	
2.20	1.022		0.974	0.980	0.989	0.986	
2.30	1.021			0.973	0.990	0.994	
2.40	1.018			0.993	0.979	0.994	
				η = 0.2755			
1.00	2.262	0.770	0.790	0.851	1.022	0.997	
1.10	1.799	0.790	0.830	0.868	1.047	1.007	
1.20	1.470	0.851	0.868	0.891	1.052	1.019	
1.30	1.232	0.890	0.910	0.936	1.039	1.030	
1.40	1.073	0.960	0.960	0.967	1.047	1.022	0.979
1.50	0.966	0.996	0.993	1.025	1.045	1.015	0.983
1.60	0.908	1.022	1.047	1.051	1.092	1.021	0.959
1.70	0.881	1.112	1.098	1.074	1.040	0.993	0.963
1.80	0.894	1.119	1.119	1.120	1.005	0.978	0.997
1.90	0.931	1.067	1.076	1.082	1.060	0.965	0.960
2.00	0.998	0.997	1.009	1.019	1.021	0.994	0.982
2.10	1.040		0.956	0.974	0.985	1.000	0.983
2.20	1.051			1.004	1.002		
2.30	1.039			0.959	0.981		
2.40	1.023			0.959	0.982		

and

$$c(R) = \frac{\eta^2 R^{-2}}{(1-\eta)^4}\left[d_1(2-R)^6 + d_2(2-R)^9 + d_3 \sin(4\pi R)\right], \quad R > 1, \quad (14)$$

where

$$d_1 = -(0{\cdot}1 + 4\eta/3), \quad d_2 = 1{\cdot}1, \quad d_3 = -\eta/15. \quad (15)$$

Using for comparison the direct c.f. obtained from the bridge function (see below), we estimate accuracy of c given by the above formulas to be about 1 per cent below the contact, while above the contact its reliability is somewhat uncertain.

Another important function not measurable in simulations is the bridge function. It can be obtained, in principle, from Eq. (7) using the data on g, c, and y. Malijevský and Labík[26,33] chose another approach based on the knowledge of the p.c.f. and thermodynamic data. They have parametrized the results as follows:

$$\begin{aligned}[B(R)]^{1/2} &= (a_1 + a_2 x)(x - a_3)(x - a_4)/(a_3 a_4), \quad 0 < x \leqq a_4 \\ &= A_1 \exp\left[-a_5(x - a_4)\right] \sin\left[A_2(x - a_4)\right]/R, \quad x \geqq a_4 \end{aligned} \quad (16)$$

where

$$\begin{aligned} x &= R - 1 \\ A_1 &= (a_1 + a_2 a_4)(a_4 - a_3)(a_4 + 1)/(A_2 a_3 a_4) \\ A_2 &= \pi/(a_6 - a_4 - 1) \\ a_1 &= \eta/(1-\eta)^2 (1{\cdot}55707 - 1{\cdot}85633\eta) \\ a_2 &= \eta/(1-\eta)(1{\cdot}28127 - 1{\cdot}82134\eta) \\ a_3 &= 0{\cdot}74480 - 0{\cdot}93453\eta \\ a_4 &= 1{\cdot}17102 - 0{\cdot}68230\eta \\ a_5 &= 0{\cdot}15975/\eta^3 \\ a_6 &= 2{\cdot}69757 - 0{\cdot}86987\eta. \end{aligned} \quad (17)$$

The bridge function given by Eq. (16) in combination with the O–Z relation (6) and Eq. (7) reproduces the simulated p.c.f. and thermodynamic properties of the fluid of hard spheres up to $n^* = 0{\cdot}94$ within their experimental accuracy. Accuracy of B itself is, however, difficult to assess. B given by Eq. (16) is consistent with c, given by Eq. (12), in the overlap region within 1 per cent.

The direct simulation data are used mainly in tests of theories, while in applications their parametrized forms, although slightly less accurate than the original data, are most frequently used. A very accurate parametrization of the p.c.f. has been proposed by Labík and Malijevský[23] but their form is rather cumbersome. Probably

the best known analytic estimate of g is that of Verlet and Weis[57]:

$$g(R, \eta) = g_{PY}(R/d, \eta_d) + \Delta g \,, \tag{18}$$

where subscript PY denotes the p.c.f. of hard spheres of a diameter d given by the Percus–Yevick theory (for a computation of g_{PY} see e.g. refs[41,47]), the diameter d is defined through the packing fraction η_d,

$$\eta_d = d^3\eta \tag{19}$$

and

$$\eta_d = \eta - \eta^2/16 \,. \tag{20}$$

The correction term Δg is given by

$$\Delta g(R/d) = \frac{A}{R} \exp\left[-Bd\left(\frac{R}{d} - 1\right)\right] \cos\left[Bd\left(\frac{R}{d} - 1\right)\right], \tag{21}$$

where

$$A/d = 0{\cdot}75\eta_d^2(1 - 0{\cdot}7117\eta_d - 0{\cdot}114\eta_d^2)(1 - \eta_d)^{-4} \tag{22}$$

$$Bd = 24(A/d)\,[\eta_d g_{PY}(R = d, \eta_d)]^{-1} \,. \tag{23}$$

The above formula reproduces the simulated values with accuracy of about 0·01 to 0·02, at densities n^* about 0·9 and higher the accuracy is slightly less. If a more accurate p.c.f. is required, one can use the values obtained from the solution of the O–Z equation coupled with the parametrized bridge function (*16*) (see Malijevský and Labík[26,33] for details).

The background c.f. has been parametrized by Henderson and Grundke[19], Ballance and Speedy[2], Boublík[7], Labík et al.[29], and quite recently again by Labík and Smith[28]. The most accurate parametrization seems that of Labík et al., but their form is, again, quite uncomfortable for applications. Next in the accuracy seems Boublík's parametrization, which also has the virtue of relative simplicity:

$$kT \ln y(R) = 2\mu(0) - \mu(R) \,, \tag{24}$$

where

$$\mu(R) = -\ln(1 - \eta) + (3R^* + 3S^* + V^*)\,\eta/(1 - \eta) + \\ + (3R^{*2} + 6S^* + 6V^*)\,\eta^2/[2(1 - \eta)^2] + V^*\eta^3(2 - \eta/3)/(1 - \eta)^3 \,. \tag{25}$$

$$R^* = 1 + 0{\cdot}5R$$

$$S^* = 1 + R$$

$$V^* = 1 + 1{\cdot}5R - 0{\cdot}125R^3 \tag{26}$$

Deviations of y given by this expression from the MC values do not exceed 5 per cent at $n^* = 0{\cdot}7$ and $R < 1$.

4. CONVEX BODY MODELS

Although these models have attracted attention for years, structural data are available only for prolate spherocylinders; the other only existing data are those on oblate spherocylinders due to Wojcik and Gubbins[59] but no tables of g_{klm} are available.

The model of prolate spherocylinders was primarily of interest for the study of nematic liquid crystals[58]. Later simulations by Nezbeda and coworkers[9,36,37] and Monson and Rigby[35] report, besides the equation of state, also various structural data. These simulations cover the elongation range $\langle 1{\cdot}4, 3{\cdot}0\rangle$ and the packing fraction range $\langle 0{\cdot}2, 0{\cdot}5\rangle$. The data available include the spherical harmonic expansion coefficients g_{klm}, surface-to-surface functions g_s, and radial slices through $g(1, 2)$.

In Table IV the listed coefficients g_{klm} and radial slices for $\gamma = 1{\cdot}4$ and $1{\cdot}6$ are due to Nezbeda[36] ($N = 192$, $N_c = 4{\cdot}6 \,.\, 10^5$, and $N_a = 600$ for $\gamma = 1{\cdot}4$ and $N = 108$, $N_c = 5{\cdot}2 \,.\, 10^5$, and $N_a = 1\,200$ for $\gamma = 1{\cdot}6$). The spherical harmonic expansion coefficients for $\gamma = 2$ and 3 given in Table V are due to Monson and Rigby[35] ($N = 108$, $N_c = 5{\cdot}4 \,.\, 10^5$) and the functions g_s given in Table VI are due to Nezbeda[36] (N, N_c, and N_a for $\gamma = 2$ are the same as those for $\gamma = 1{\cdot}6$). Accuracy of the spherical harmonic expansion coefficients and of the surface-to-surface correlation functions was not explicitly given in the original papers but this is estimated to be about 4 per cent. Accuracy of the slices is evidently much lower. Main problems associated with this sort of simulations are the choice of the size of cones $(\pm\Delta\vartheta, \pm\Delta\phi)$ into which the solid angle is divided and the proper evaluation of the actual accessible volume at small separations. In the reported simulations the values $\Delta\vartheta = \Delta\phi = 8°$ were used. With the above given number of generated configurations it was not possible to obtain even any reasonable information on the end-to-end configuration and the results for the parallel configuration at small separations are also questionable. We list here therefore only the results for the crossed and T-shaped configurations whose accuracy is between 10 and 15 per cents.

5. FUSED HARD SPHERE MODELS

Homonuclear Diatomics

The fluid of homonuclear diatomics is the hard body system most intensively investigated next to hard spheres. The first simulations were apparently performed by Freasier[15] but he reported only the equation of state without mentioning any results for the structure. Although the literature on this system is quite ample (for references see e.g. Levesque et al.[31]), tables of the coefficients g_{klm} can be found only in a paper

TABLE IV

Fluids of hard prolate spherocylinders: spherical harmonic expansion coefficients and radial slices through g(1,2) at the crossed (C) and T-shaped (T) configurations

R	g_{000}	g_{200}	g_{220}	g_{221}	g_{222}	g_{400}	g_C	g_T
			$\gamma = 1.4, \quad \eta = 0.3142$					
1.00	0.044	-0.047	0.051	-0.002	-0.011	0.043		
1.08	0.439	-0.400	0.357	-0.045	-0.011	0.242	2.61	
1.16	1.045	-0.624	0.227	-0.114	0.002	0.122	2.24	
1.24	1.575	-0.380	-0.398	-0.076	-0.008	0.032	1.71	2.48
1.32	1.694	-0.024	-0.303	0.001	0.008	-0.081	1.37	2.25
1.40	1.574	0.169	-0.004	0.023	0.011	-0.006	1.24	1.80
1.48	1.348	0.135	0.031	0.015	0.005	-0.001	1.13	1.35
1.56	1.165	0.116	0.019	0.020	0.007	0.006	0.98	1.22
1.64	1.048	0.089	0.014	0.003	0.006	-0.008	0.82	1.10
1.72	0.964	0.067	0.007	0.015	0.007	-0.017	0.81	0.93
1.80	0.902	0.049	0.013	0.008	-0.006	-0.014	0.81	0.86
1.88	0.868	0.036	0.016	0.007	0.001	-0.013	0.77	0.87
1.96	0.864	0.011	0.006	0.000	0.000	-0.009	0.82	0.87
2.04	0.870	-0.000	0.011	-0.002	0.005	-0.009	0.92	0.86
2.12	0.898	-0.025	0.007	-0.002	0.001	0.003	0.88	0.85
2.20	0.936	-0.026	0.013	-0.006	0.006	-0.001	1.01	0.95
2.28	0.976	-0.041	0.003	-0.000	0.004	0.008	1.02	0.95
2.36	1.018	-0.030	-0.006	-0.003	0.000	0.003	1.06	0.94
2.44	1.043	-0.022	-0.005	0.001	0.002	0.001	1.07	0.98
2.52	1.055	-0.008	-0.006	0.002	0.005	0.001	1.11	1.11
2.60	1.054	0.000	-0.005	-0.001	0.002	-0.001	0.96	1.15
2.68	1.046	0.006	-0.005	0.000	0.002	-0.001	1.05	1.02
2.76	1.027	0.014	-0.005	-0.002	0.001	0.001	0.97	1.04
2.84	1.010	0.014	-0.002	-0.001	0.004	-0.002	0.97	1.06
2.92	0.998	0.011	0.000	-0.003	0.000	-0.005	1.04	1.03
3.00	0.993	0.011	0.000	0.002	-0.001	-0.001	0.99	0.97

TABLE IV
(Continued)

R	g_{000}	g_{200}	g_{220}	g_{221}	g_{222}	g_{400}	g_C	g_T
				$\gamma = 1.6$, $\eta = 0.2948$				
1.0238	0.086	-0.092	0.098	-0.004	-0.028	0.082	2.67	
1.1190	0.449	-0.401	0.356	-0.063	-0.028	0.223	1.88	
1.2143	0.887	-0.568	0.293	-0.145	0.005	0.078	2.04	
1.3095	1.316	-0.412	-0.271	-0.138	-0.008	0.028	1.14	
1.4048	1.465	-0.168	-0.408	-0.051	0.007	-0.063	1.57	2.13
1.5000	1.467	0.008	-0.192	0.019	0.014	-0.078	1.12	1.56
1.5952	1.326	0.156	0.021	0.024	0.005	0.004	0.78	1.41
1.6905	1.153	0.139	0.029	0.023	0.003	-0.004	1.08	1.31
1.7857	1.049	0.110	0.021	0.017	-0.002	-0.002	0.84	1.31
1.8810	0.962	0.067	0.021	0.009	-0.001	-0.016	0.71	0.91
1.9762	0.914	0.050	0.021	0.005	-0.006	-0.010	1.03	0.90
2.0714	0.896	0.020	0.033	0.007	-0.003	0.000	0.87	0.81
2.1667	0.902	-0.002	0.035	-0.006	-0.004	0.000	0.93	0.72
2.2619	0.922	-0.020	0.010	0.003	-0.004	-0.002	1.00	0.96
2.3571	0.944	-0.029	0.009	0.003	-0.003	-0.003	1.10	0.93
2.4524	0.981	-0.034	0.001	0.001	0.000	0.008	1.14	1.03
2.5476	1.002	-0.025	-0.006	-0.002	-0.005	0.003	1.05	1.03
2.6429	1.017	-0.015	-0.013	0.003	0.004	-0.005	1.09	1.11
2.7381	1.022	-0.014	-0.016	-0.003	-0.006	-0.001	1.09	1.13
2.8333	1.028	-0.002	-0.002	0.003	-0.002	-0.003	1.10	1.03
2.9286	1.029	0.003	-0.001	0.001	0.002	0.001	1.09	1.03
3.0238	1.021	0.009	-0.004	-0.002	0.005	-0.002	0.96	1.08
3.1190	1.008	0.012	0.003	0.002	0.002	-0.002	0.89	1.04
3.2143	1.004	0.007	0.002	0.004	-0.003	0.002	0.89	1.00
3.3095	0.993	0.009	-0.002	0.005	0.000	-0.006	1.00	0.97
3.4048	0.991	0.007	-0.006	0.003	-0.000	-0.003	0.99	1.01

TABLE IV
(Continued)

R	g_{000}	g_{200}	g_{220}	g_{221}	g_{222}	g_{400}	g_C	g_T
				$\gamma = 1.6, \quad \eta = 0.3873$				
1.0217	0.133	-0.142	0.153	-0.005	-0.052	0.129	4.60	
1.1087	0.608	-0.558	0.510	-0.082	-0.027	0.334	3.04	
1.1957	1.044	-0.718	0.416	-0.184	-0.005	0.139	2.47	
1.2826	1.489	-0.547	-0.214	-0.211	0.006	-0.011	1.86	
1.3696	1.688	-0.194	-0.637	-0.105	0.016	-0.016	0.95	2.83
1.4565	1.600	0.101	-0.420	0.011	-0.002	-0.122	1.02	2.32
1.5435	1.403	0.294	-0.034	0.045	-0.003	-0.043	0.87	1.79
1.6304	1.178	0.251	0.090	0.050	0.001	0.011	0.60	1.12
1.7174	0.991	0.186	0.069	0.033	0.005	-0.009	0.64	1.07
1.8043	0.875	0.131	0.049	0.026	-0.000	-0.005	0.53	0.86
1.8913	0.819	0.081	0.057	0.018	-0.005	-0.004	0.64	0.70
1.9783	0.809	0.040	0.045	0.007	-0.001	0.000	0.53	0.75
2.0652	0.836	-0.008	0.052	0.006	-0.005	0.001	0.94	0.67
2.1522	0.871	-0.047	0.047	0.001	-0.008	0.007	1.09	0.80
2.2391	0.938	-0.069	0.038	-0.004	-0.002	0.015	1.22	0.81
2.3261	0.993	-0.066	0.007	-0.003	-0.007	0.014	1.30	1.03
2.4130	1.035	-0.062	-0.018	-0.011	0.000	0.011	1.16	1.05
2.5000	1.068	-0.044	-0.025	-0.011	-0.004	-0.004	1.08	1.05
2.5870	1.076	-0.017	-0.025	-0.007	0.001	-0.006	1.01	0.96
2.6739	1.064	0.004	-0.023	-0.005	-0.001	0.007	0.95	1.14
2.7609	1.049	0.011	-0.020	-0.006	-0.003	0.009	0.96	1.15
2.8478	1.025	0.020	-0.013	0.004	0.006	-0.001	0.92	1.10
2.9348	0.995	0.016	-0.006	0.003	-0.005	-0.002	0.99	1.02
3.0217	0.994	0.015	-0.002	0.002	0.000	-0.007	0.87	1.02
3.1087	0.975	0.012	0.002	-0.001	0.001	-0.008	0.93	1.03
3.1957	0.977	0.001	0.015	0.002	-0.001	0.006	1.05	1.03

TABLE V
Fluids of hard prolate spherocylinders: spherical harmonic expansion coefficients

R	g_{000}	g_{200}	g_{220}	g_{221}	g_{222}	g_{400}
			$\gamma = 2, \quad \eta = 0.3$			
1.025	0.098	-0.105	0.112	-0.004	-0.023	0.095
1.075	0.269	-0.268	0.268	-0.026	-0.064	0.202
1.125	0.407	-0.373	0.349	-0.065	-0.058	0.218
1.175	0.545	-0.458	0.393	-0.108	-0.035	0.197
1.225	0.663	-0.504	0.390	-0.145	-0.029	0.138
1.275	0.773	-0.519	0.341	-0.183	-0.006	0.054
1.325	0.924	-0.551	0.280	-0.214	-0.008	-0.011
1.375	1.019	-0.498	0.140	-0.238	-0.000	-0.090
1.425	1.112	-0.429	-0.009	-0.232	0.005	-0.128
1.475	1.219	-0.351	-0.200	-0.219	0.017	-0.083
1.525	1.308	-0.262	-0.380	-0.202	0.012	-0.009
1.575	1.295	-0.192	-0.418	-0.153	0.014	-0.041
1.625	1.287	-0.122	-0.388	-0.110	0.010	-0.047
1.675	1.288	-0.057	-0.344	-0.078	0.012	-0.091
1.725	1.245	0.021	-0.306	-0.030	0.015	-0.105
1.775	1.235	0.087	-0.217	-0.007	0.018	-0.098
1.825	1.202	0.123	-0.119	0.002	0.020	-0.068
1.875	1.158	0.159	-0.041	0.020	0.019	-0.044
1.925	1.132	0.175	0.046	0.025	0.016	-0.031
1.975	1.075	0.161	0.056	0.017	-0.001	0.012
2.075	1.010	0.116	0.076	0.010	0.003	0.003
2.175	0.971	0.064	0.068	0.005	-0.003	0.006
2.275	0.951	0.029	0.069	-0.001	-0.001	0.014
2.375	0.943	-0.003	0.055	-0.013	-0.003	0.003
2.475	0.952	-0.041	0.038	-0.013	0.002	0.008
2.575	0.967	-0.045	0.026	-0.012	0.000	0.002
2.675	0.982	-0.052	0.011	-0.014	0.010	-0.004
2.775	1.004	-0.032	-0.014	-0.005	-0.004	-0.001
2.875	1.012	-0.036	-0.006	-0.002	-0.003	-0.005
2.975	1.019	-0.023	-0.024	-0.002	-0.002	-0.004

TABLE V
(Continued)

R	g_{000}	g_{200}	g_{220}	g_{221}	g_{222}	g_{400}
			$\gamma = 2, \quad \eta = 0.4$			
1.025	0.198	-0.210	0.224	-0.010	-0.049	0.188
1.075	0.513	-0.512	0.512	-0.058	-0.039	0.387
1.125	0.683	-0.628	0.584	-0.116	-0.044	0.374
1.175	0.790	-0.661	0.560	-0.178	0.007	0.279
1.225	0.915	-0.686	0.516	-0.229	0.001	0.170
1.275	0.997	-0.650	0.399	-0.264	0.013	0.039
1.325	1.088	-0.606	0.263	-0.281	0.007	-0.058
1.375	1.184	-0.528	0.076	-0.288	-0.005	-0.153
1.425	1.239	-0.416	-0.149	-0.266	0.002	-0.156
1.475	1.332	-0.297	-0.410	-0.238	-0.005	-0.097
1.525	1.366	-0.158	-0.600	-0.159	-0.006	0.036
1.575	1.373	-0.056	-0.609	-0.095	-0.001	-0.002
1.625	1.324	0.008	-0.530	-0.049	-0.001	-0.058
1.675	1.268	0.081	-0.432	0.007	0.002	-0.102
1.725	1.217	0.126	-0.328	0.041	0.011	-0.117
1.775	1.165	0.179	-0.200	0.067	0.013	-0.090
1.825	1.122	0.248	-0.042	0.068	0.006	-0.067
1.875	1.062	0.252	0.067	0.078	0.003	-0.039
1.925	1.017	0.267	0.172	0.070	0.014	0.008
1.975	0.962	0.251	0.193	0.057	-0.003	0.037
2.075	0.913	0.139	0.183	0.029	0.001	0.028
2.175	0.900	0.038	0.165	0.003	-0.001	0.022
2.275	0.912	-0.040	0.125	-0.003	-0.006	0.029
2.375	0.948	-0.067	0.082	-0.012	-0.005	0.016
2.475	1.000	-0.074	0.022	-0.019	-0.015	0.004
2.575	1.033	-0.051	-0.028	-0.024	-0.012	0.007
2.675	1.046	-0.022	-0.048	-0.027	-0.006	-0.001
2.775	1.040	-0.001	-0.051	-0.016	-0.009	-0.019
2.875	1.029	0.005	-0.035	0.002	-0.000	-0.012
2.975	1.018	0.019	-0.028	0.004	0.000	-0.014

TABLE V
(Continued)

R	g_{000}	g_{200}	g_{220}	g_{221}	g_{222}	g_{400}
			$\gamma = 2, \quad \eta = 0.5$			
1.025	0.383	-0.408	0.433	-0.020	-0.085	0.363
1.075	0.801	-0.795	0.795	-0.092	-0.088	0.592
1.125	0.956	-0.859	0.790	-0.184	-0.049	0.468
1.178	0.982	-0.797	0.656	-0.249	-0.013	0.290
1.225	1.030	-0.724	0.511	-0.309	-0.003	0.086
1.275	1.088	-0.622	0.329	-0.339	-0.040	-0.124
1.325	1.165	-0.537	0.126	-0.370	-0.031	-0.254
1.375	1.279	-0.447	-0.116	-0.358	-0.015	-0.314
1.425	1.383	-0.334	-0.410	-0.312	-0.003	-0.278
1.475	1.502	-0.177	-0.752	-0.213	-0.019	-0.128
1.525	1.536	0.011	-1.014	-0.128	0.016	0.046
1.575	1.467	0.081	-0.922	-0.019	0.015	0.022
1.625	1.341	0.151	-0.729	0.057	0.028	-0.045
1.675	1.220	0.183	-0.532	0.096	0.020	-0.084
1.725	1.125	0.235	-0.339	0.114	0.024	-0.092
1.775	1.032	0.284	-0.155	0.136	0.018	-0.074
1.825	0.960	0.335	-0.004	0.142	0.016	-0.022
1.875	0.890	0.324	0.160	0.144	0.019	0.011
1.925	0.864	0.291	0.266	0.127	0.025	0.073
1.975	0.834	0.209	0.319	0.107	0.030	0.100
2.075	0.829	0.002	0.271	0.044	0.023	0.103
2.175	0.907	-0.129	0.231	0.005	0.018	0.096
2.275	0.968	-0.168	0.144	-0.023	0.007	0.050
2.375	1.007	-0.141	0.025	-0.040	0.000	0.016
2.475	1.048	-0.074	-0.084	-0.032	0.009	-0.009
2.575	1.065	-0.013	-0.143	-0.008	0.016	-0.012
2.675	1.055	0.035	-0.147	0.011	0.018	-0.020
2.775	1.043	0.069	-0.087	0.017	0.024	-0.045
2.875	1.011	0.067	-0.011	0.013	0.017	-0.041
2.975	0.990	0.046	0.035	0.004	0.003	-0.014

TABLE V
(Continued)

R	g_{000}	g_{200}	g_{220}	g_{221}	g_{222}	g_{400}
			$\gamma = 3, \quad \eta = 0.3$			
1.025	0.122	-0.130	0.139	-0.006	-0.033	0.116
1.075	0.311	-0.309	0.311	-0.031	-0.083	0.230
1.125	0.464	-0.432	0.402	-0.072	-0.090	0.268
1.175	0.606	-0.526	0.465	-0.114	-0.123	0.259
1.225	0.660	-0.530	0.435	-0.148	-0.119	0.190
1.275	0.714	-0.537	0.414	-0.184	-0.102	0.138
1.325	0.762	-0.522	0.377	-0.213	-0.098	0.057
1.375	0.797	-0.518	0.352	-0.233	-0.076	0.023
1.425	0.846	-0.504	0.316	-0.245	-0.095	-0.036
1.475	0.848	-0.466	0.269	-0.267	-0.063	-0.078
1.525	0.869	-0.418	0.216	-0.275	-0.062	-0.150
1.575	0.892	-0.410	0.187	-0.268	-0.068	-0.156
1.625	0.879	-0.343	0.132	-0.263	-0.033	-0.198
1.675	0.926	-0.333	0.081	-0.269	-0.012	-0.211
1.725	0.928	-0.302	0.037	-0.256	-0.025	-0.203
1.775	0.961	-0.248	-0.028	-0.247	-0.025	-0.214
1.825	0.972	-0.194	-0.085	-0.237	-0.031	-0.208
1.875	1.001	-0.203	-0.134	-0.205	-0.027	-0.155
1.925	1.030	-0.149	-0.211	-0.187	-0.009	-0.131
1.975	1.052	-0.089	-0.276	-0.161	-0.006	-0.072
2.075	1.083	-0.026	-0.325	-0.092	-0.006	-0.006
2.175	1.083	0.004	-0.296	-0.047	-0.001	-0.001
2.275	1.051	-0.009	-0.194	-0.004	-0.003	-0.013
2.375	1.027	0.016	-0.138	0.024	0.005	-0.009
2.475	1.037	0.016	-0.051	0.058	0.003	-0.038
2.575	1.020	0.030	-0.002	0.050	-0.002	-0.030
2.675	1.029	0.028	0.050	0.046	-0.004	-0.028
2.775	1.016	0.018	0.071	0.042	-0.010	-0.019
2.875	1.021	0.039	0.101	0.023	-0.004	0.001
2.975	1.015	0.027	0.099	0.023	-0.006	0.015

TABLE VI

Fluids of hard prolate spherocylinders: average surface-to-surface correlation functions

γ=1.4, η=0.3142		γ=1.6, η=0.2948		γ=1.6, η=0.3873		γ=2.0, η=0.3879	
s	g_s	s	g_s	s	g_s	s	g_s
0.02	2.539	0.0238	2.362	0.0217	3.302	0.0238	3.435
0.08	2.149	0.0714	2.120	0.0652	2.791	0.0714	2.843
0.16	1.773	0.1190	1.896	0.1087	2.363	0.1190	2.375
0.24	1.482	0.1667	1.739	0.1522	2.023	0.1667	2.040
0.32	1.280	0.2143	1.586	0.1957	1.769	0.2143	1.720
0.40	1 122	0.2619	1.458	0.2391	1.543	0.2619	1.510
0.48	1.012	0.3095	1.350	0.2826	1.368	0.3095	1.331
0.56	0.928	0.3571	1.254	0.3261	1.218	0.3571	1.186
0.64	0.876	0.4048	1.166	0.3696	1.100	0.4048	1.069
0.72	0.850	0.4524	1.103	0.4130	1.018	0.4524	0.983
0.80	0.850	0.5000	1.036	0.4565	0.934	0.5000	0.910
0.88	0.868	0.5952	0.957	0.5000	0.887	0.5476	0.846
0.96	0.896	0.6905	0.898	0.5435	0.834	0.5952	0.817
1.04	0.944	0.7857	0.881	0.5870	0.801	0.6429	0.786
1.12	0.991	0.8810	0.869	0.6304	0.782	0.6905	0.772
1.20	1.036	0.9762	0.900	0.6739	0.771	0.7381	0.768
1.28	1.055	1.0714	0.939	0.7174	0.765	0.7857	0.778
1.36	1.064	1.1667	0.976	0.7609	0.770	0.8333	0.788
1.44	1.061	1.2619	1.010	0.8043	0.789	0.8810	0.817
1.52	1.043	1.3571	1.031	0.8913	0.841	0.9286	0.849
1.60	1.020	1.4524	1.032	0.9783	0.913	0.9762	0.894
1.68	1.008	1.5476	1.036	1.0652	1.014	1.0238	0.944
1.76	0.994	1.6429	1.025	1.1522	1.073	1.0714	0.994
1.92	0.982	1.7381	1.025	1.2391	1.092	1.1667	1.059
2.08	0.980	1.8333	1.010	1.3261	1.089	1.2619	1.088
2.24	0.990	1.9286	1.001	1.4130	1.076	1.3571	1.076
2.40	1.002			1.5000	1.048	1.4524	1.053
2 56	1.008			1.5870	1.027	1.5476	1.023

by Streett and Tildesley[51]; MC results for G_{ss} (shown in graphs only) appear first in a paper by Chandler et al.[11]. Elongations L considered since by various authors[31] have varied within the range $\langle 0, 1 \rangle$ with larger elongations (about 0·8 and more) having only a certain theoretical importance. It seems that the elongations $L = 0{\cdot}2$, 0·4, and 0·6 may be good representatives of models of the greatest interest and results only for them are therefore listed.

Comparison of the simulation results on g_{klm} of various authors for $L = 0{\cdot}6$ at higher densities indicates that the accuracy of the extensive data by Streett and Tildesley[51] is only fair (one reason may be an improper sampling of the orientational space used by these authors in their simulations). For the presentation in this compilation we have therefore chosen the latest simulation results by Labík et al.[30] ($N = 256$, $N_c = (3-5) \cdot 10^6$, $N_c/N_a = 2\,560$) which are very accurate (the leading spherical harmonic expansion coefficient, g_{000}, is accurate within 1 per cent, the scatter of higher coefficients is about 0·003) and provide the structural properties at four densities for each elongation. These results are listed in Table VII (for the diatomics of the smallest elongation, $L = 0{\cdot}2$, we list the data at the highest density only which we believe is sufficient). We only remind in passing that the average site–site c.f. G_{ss} ($\equiv G_{000}$) exhibits a cusp at $r = L + 1$.

For $L = 0{\cdot}6$ and $n^* = 0{\cdot}5$ Cummings et al.[13] performed painstaiking simulations ($N = 144$, $N_c = 18 \cdot 10^6$, $N_a = 3{\cdot}6 \cdot 10^6$) to obtain, in addition to the average site–site p.c.f. and few spherical harmonic expansion coefficients g_{klm}, radial slices through the full p.c.f. The fixed angular intervals were set to $\Delta\vartheta = \Delta\phi = 10°$ and the overall accuracy of the slices is abut 5 per cent for small R. With respect to the enormous number of the generated configurations the data on g_{klm} and G_{ss} may also serve as a benchmark of accuracy of other data. Similarly, Labík and Malijevský[25] carried out simulations ($N = 256$, $N_c = 2 \cdot 10^5$, 10^6, and $3 \cdot 10^6$ for $n^* = 0{\cdot}2$, 0·3, and 0·4, respectively; $N_c/N_a = 1\,024$) for the same elongation to obtain the radial slices through $y(1, 2)$ (it turned out that the density 0·5 was too high to accomplish this sort of simulations). The above two simulations are quite unique and provide the only available information on the structure of fluids of fused hard spheres beyond various angle averages and spherical harmonic expansion coefficients; they are listed in Tables VIII and IX.

Heteronuclear Diatomics

This model, in addition to L, is characterized also by the ratio σ_B/σ_A ($= \sigma_B$ because $\sigma_A = 1$) which makes its systematic investigation complicated. Streett and Tildesley[52] reported results ($N = 256$, $N_c = 2 \cdot 10^6$) for the average site–site c.f. $G_{\alpha\beta}$ for a number systems at one density and for one system ($L = 0{\cdot}346$, $\sigma_B = 0{\cdot}675$) at several densities. Accuracy of these data is about 3 per cent. Nezbeda et al.[39] considered a system of the significantly larger asymmetry ($L = 0{\cdot}625$, $\sigma_B = 0{\cdot}5$) at

TABLE VII
Fluids of hard homonuclear diatomics: spherical harmonic expansion coefficients

R	g_{000}	g_{200}	g_{220}	g_{221}	g_{222}	g_{400}	G_{000}	G_{100}
			L = 0.2,	η = 0.4712				
1.000	0.041	-0.045	0.049	-0.001	-0.008	0.043	1.591	-1.189
1.025	0.371	-0.384	0.396	-0.016	-0.004	0.321	1.698	-1.083
1.050	0.909	-0.824	0.724	-0.055	0.005	0.493	1.788	-0.942
1.075	1.594	-1.119	0.623	-0.104	0.006	0.338	1.869	-0.792
1.100	2.351	-1.034	-0.183	-0.118	0.014	0.195	1.927	-0.624
1.125	2.854	-0.639	-0.879	-0.074	0.009	0.029	1.987	-0.441
1.150	3.024	-0.154	-0.850	-0.018	0.000	-0.169	2.056	-0.253
1.175	2.921	0.275	-0.318	0.015	0.003	-0.146	2.138	-0.053
1.200	2.621	0.443	0.060	0.024	0.005	-0.013	2.188	0.144
1.225	2.269	0.372	0.064	0.023	-0.002	-0.002	2.031	0.234
1.250	1.961	0.312	0.065	0.012	0.004	-0.008	1.848	0.285
1.275	1.715	0.262	0.043	0.015	0.005	-0.002	1.686	0.312
1.300	1.504	0.232	0.038	0.012	0.003	-0.017	1.541	0.333
1.325	1.337	0.195	0.032	0.011	-0.003	-0.012	1.409	0.331
1.350	1.192	0.161	0.026	0.007	0.000	-0.021	1.287	0.323
1.375	1.075	0.140	0.020	0.009	-0.003	-0.013	1.173	0.299
1.400	0.981	0.116	0.018	0.010	-0.003	-0.017	1.065	0.257
1.425	0.909	0.102	0.015	0.006	-0.006	-0.017	0.976	0.212
1.450	0.838	0.094	0.019	0.003	-0.002	-0.025	0.899	0.175
1.475	0.782	0.082	0.010	0.006	-0.002	-0.019	0.831	0.145
1.500	0.740	0.065	0.013	0.003	-0.001	-0.021	0.784	0.122
1.525	0.701	0.056	0.005	0.008	-0.002	-0.018	0.741	0.094
1.550	0.672	0.054	0.008	0.004	-0.004	-0.022	0.706	0.073
1.575	0.652	0.040	0.007	0.003	0.000	-0.018	0.685	0.059
1.600	0.637	0.038	0.006	0.001	0.003	-0.020	0.666	0.042
1.625	0.627	0.028	0.009	0.000	0.003	-0.018	0.658	0.028
1.650	0.627	0.018	0.014	0.002	0.001	-0.019	0.653	0.016
1.675	0.632	0.013	0.009	-0.001	0.003	-0.016	0.656	0.002
1.700	0.635	0.010	0.008	0.000	-0.003	-0.018	0.660	-0.008

TABLE VII
(Continued)

R	g_{000}	g_{200}	g_{220}	g_{221}	g_{222}	g_{400}	G_{000}	G_{100}
1.725	0.648	0.001	0.010	-0.001	0.003	-0.016	0.673	-0.020
1.750	0.659	-0.004	0.007	0.001	-0.001	-0.013	0.689	-0.031
1.775	0.685	-0.011	0.006	0.001	0.000	-0.011	0.711	-0.043
1.800	0.708	-0.020	0.011	-0.001	0.000	-0.009	0.743	-0.053
1.825	0.743	-0.025	0.009	-0.004	-0.001	-0.012	0.774	-0.063
1.850	0.786	-0.035	0.011	-0.001	-0.001	-0.005	0.812	-0.074
1.875	0.827	-0.041	0.015	-0.001	-0.003	-0.004	0.849	-0.082
1.900	0.874	-0.051	0.012	-0.001	0.003	-0.005	0.892	-0.087
1.925	0.925	-0.055	0.005	-0.001	0.000	0.000	0.933	-0.088
1.950	0.969	-0.056	0.005	-0.001	0.001	0.004	0.974	-0.090
1.975	1.021	-0.057	0.009	-0.003	0.001	0.007	1.017	-0.088
2.000	1.057	-0.060	0.006	-0.004	-0.001	0.010	1.060	-0.087
2.050	1.141	-0.057	0.001	-0.005	0.000	0.019	1.132	-0.079
2.100	1.202	-0.053	-0.002	-0.004	-0.001	0.019	1.187	-0.061
2.150	1.244	-0.037	-0.010	-0.004	-0.001	0.017	1.218	-0.040
2.200	1.264	-0.018	-0.015	-0.004	-0.003	0.013	1.227	-0.013
2.250	1.246	0.002	-0.014	0.000	0.000	0.009	1.210	0.015
2.300	1.205	0.022	-0.013	0.000	0.001	0.005	1.175	0.040
2.350	1.146	0.033	-0.007	-0.002	-0.002	-0.001	1.121	0.056
2.400	1.070	0.040	-0.005	0.000	0.001	-0.002	1.064	0.065
2.450	1.000	0.035	-0.002	0.004	-0.001	-0.002	1.008	0.064
2.500	0.946	0.034	-0.003	0.000	-0.002	-0.009	0.958	0.056
2.550	0.902	0.028	0.001	0.002	0.002	-0.007	0.920	0.043
2.600	0.879	0.023	0.004	0.001	0.003	-0.008	0.893	0.030
2.650	0.862	0.014	0.003	-0.001	0.000	-0.006	0.879	0.015
2.700	0.860	0.008	0.006	0.002	0.000	-0.008	0.877	0.003
2.750	0.873	-0.002	0.005	-0.001	-0.001	-0.007	0.889	-0.012
2.800	0.896	-0.005	0.004	0.000	0.000	-0.004	0.909	-0.023
2.850	0.930	-0.015	0.004	0.001	0.000	-0.003	0.936	-0.030
2.900	0.960	-0.018	0.002	-0.003	0.001	-0.002	0.966	-0.035
2.950	0.997	-0.019	0.003	-0.001	-0.002	-0.001	1.000	-0.036
3.000	1.033	-0.015	0.001	-0.002	0.002	0.003	1.028	-0.033

TABLE VII
(Continued)

R	g_{000}	g_{200}	g_{220}	g_{221}	g_{222}	g_{400}	G_{000}	G_{100}
			L = 0.4,	η = 0.2094				
0.975	0.002	-0.002	0.002	0.000	-0.003	0.002		
1.000	0.025	-0.027	0.029	-0.001	-0.018	0.025	0.661	-0.453
1.025	0.090	-0.094	0.099	-0.006	-0.019	0.082	0.705	-0.450
1.050	0.173	-0.173	0.172	-0.016	-0.016	0.132	0.746	-0.438
1.075	0.290	-0.270	0.248	-0.032	-0.023	0.172	0.793	-0.429
1.100	0.416	-0.357	0.293	-0.049	-0.008	0.181	0.831	-0.415
1.125	0.559	-0.428	0.293	-0.068	-0.004	0.157	0.876	-0.394
1.150	0.707	-0.463	0.223	-0.083	-0.004	0.110	0.909	-0.372
1.175	0.891	-0.479	0.094	-0.090	-0.002	0.080	0.951	-0.349
1.200	1.054	-0.443	-0.091	-0.094	-0.006	0.076	0.980	-0.319
1.225	1.180	-0.389	-0.218	-0.076	-0.006	0.050	1.022	-0.292
1.250	1.297	-0.327	-0.293	-0.054	0.009	0.010	1.055	-0.258
1.275	1.344	-0.230	-0.325	-0.042	0.000	-0.027	1.089	-0.230
1.300	1.428	-0.153	-0.290	-0.029	0.013	-0.064	1.121	-0.192
1.325	1.443	-0.066	-0.222	-0.004	-0.010	-0.068	1.154	-0.155
1.350	1.456	0.007	-0.127	0.004	0.003	-0.048	1.192	-0.117
1.375	1.446	0.059	-0.046	0.012	0.001	-0.016	1.226	-0.078
1.400	1.411	0.080	0.004	0.007	-0.003	-0.001	1.252	-0.036
1.425	1.365	0.075	0.001	0.000	-0.003	0.008	1.245	-0.020
1.450	1.334	0.076	0.015	0.003	-0.003	0.005	1.231	-0.002
1.475	1.303	0.072	0.009	0.007	-0.004	-0.003	1.216	0.013
1.500	1.267	0.063	0.006	0.006	0.001	0.009	1.201	0.020
1.525	1.237	0.058	-0.002	0.007	0.000	-0.002	1.184	0.033
1.550	1.210	0.059	-0.004	0.007	0.002	-0.001	1.163	0.040
1.575	1.189	0.050	0.001	0.007	0.006	-0.008	1.153	0.054
1.600	1.160	0.050	0.008	0.005	0.002	-0.002	1.141	0.060
1.625	1.135	0.052	0.011	0.000	0.001	-0.003	1.129	0.063
1.650	1.114	0.050	0.003	0.008	0.004	-0.007	1.108	0.068
1.675	1.087	0.046	0.000	0.007	-0.003	0.005	1.098	0.071
1.700	1.076	0.040	0.004	0.002	-0.003	-0.006	1.080	0.073

TABLE VII
(Continued)

R	g_{000}	g_{200}	g_{220}	g_{221}	g_{222}	g_{400}	G_{000}	G_{100}
1.725	1.061	0.040	0.005	0.007	0.002	-0.005	1.071	0.073
1.750	1.031	0.041	-0.004	0.004	-0.003	-0.008	1.057	0.071
1.775	1.025	0.037	0.001	0.000	-0.002	-0.002	1.041	0.066
1.800	1.016	0.035	-0.010	0.004	-0.004	-0.003	1.027	0.062
1.825	0.999	0.033	0.012	0.003	0.002	-0.008	1.014	0.058
1.850	0.987	0.029	-0.001	0.000	0.001	-0.007	1.003	0.053
1.875	0.981	0.025	0.006	0.001	0.004	0.003	0.996	0.051
1.900	0.968	0.025	0.002	-0.001	0.002	-0.003	0.987	0.043
1.925	0.963	0.017	0.005	-0.002	0.000	-0.005	0.979	0.037
1.950	0.962	0.024	0.007	0.001	-0.008	0.000	0.973	0.035
1.975	0.954	0.020	0.003	0.007	0.001	-0.005	0.969	0.028
2.000	0.945	0.015	0.002	0.003	-0.002	-0.001	0.968	0.021
2.050	0.940	0.012	0.008	0.006	0.001	-0.002	0.961	0.017
2.100	0.941	0.007	0.007	0.005	0.000	-0.005	0.959	0.005
2.150	0.947	-0.008	0.003	-0.001	0.001	0.001	0.962	-0.001
2.200	0.947	-0.005	0.010	0.000	0.001	0.003	0.967	-0.007
2.250	0.960	-0.012	-0.005	-0.003	0.001	0.000	0.969	-0.011
2.300	0.971	-0.007	0.001	0.002	-0.001	-0.001	0.978	-0.014
2.350	0.979	-0.007	-0.001	0.001	-0.002	0.000	0.986	-0.015
2.400	0.991	-0.012	0.001	0.002	-0.002	0.003	0.989	-0.015
2.450	0.999	-0.012	0.000	0.002	-0.001	-0.002	0.999	-0.015
2.500	1.005	-0.007	-0.001	-0.001	-0.001	0.002	1.004	-0.013
2.550	1.011	-0.005	-0.005	0.002	-0.002	-0.001	1.007	-0.010
2.600	1.014	-0.010	0.002	0.002	-0.001	-0.001	1.011	-0.010
2.650	1.016	-0.005	-0.004	0.000	0.000	-0.001	1.012	-0.006
2.700	1.019	-0.002	0.000	0.000	-0.001	0.001	1.014	-0.005
2.750	1.022	-0.003	-0.001	0.002	0.002	-0.001	1.013	-0.001
2.800	1.014	0.000	-0.001	-0.001	0.000	0.002	1.016	0.002
2.850	1.016	0.002	0.000	0.000	-0.003	0.003	1.013	0.001
2.900	1.014	0.002	-0.001	0.001	-0.003	0.003	1.007	0.011
2.950	1.010	0.000	0.000	-0.004	0.001	0.001	0.981	0.041
3.000	1.005	0.004	-0.002	0.002	0.000	-0.001	0.941	0.089

TABLE VII
(Continued)

R	g_{000}	g_{200}	g_{220}	g_{221}	g_{222}	g_{400}	G_{000}	G_{100}
			L = 0.4,	η = 0.3142				
0.975	0.004	-0.004	0.005	0.000	-0.007	0.004		
1.000	0.042	-0.045	0.049	-0.002	-0.029	0.043	0.975	-0.655
1.025	0.144	-0.151	0.158	-0.010	-0.023	0.130	1.009	-0.624
1.050	0.278	-0.277	0.275	-0.026	-0.020	0.210	1.042	-0.590
1.075	0.436	-0.407	0.375	-0.048	-0.017	0.260	1.069	-0.551
1.100	0.614	-0.523	0.427	-0.074	-0.021	0.260	1.102	-0.517
1.125	0.787	-0.597	0.403	-0.098	-0.013	0.210	1.131	-0.474
1.150	0.987	-0.639	0.299	-0.121	-0.001	0.142	1.153	-0.431
1.175	1.201	-0.622	0.079	-0.127	0.005	0.097	1.181	-0.387
1.200	1.392	-0.555	-0.178	-0.122	-0.001	0.093	1.197	-0.341
1.225	1.540	-0.464	-0.363	-0.105	0.015	0.060	1.222	-0.296
1.250	1.641	-0.358	-0.458	-0.074	0.013	0.007	1.249	-0.251
1.275	1.701	-0.226	-0.481	-0.053	0.009	-0.054	1.263	-0.201
1.300	1.731	-0.109	-0.417	-0.026	0.007	-0.095	1.287	-0.153
1.325	1.721	0.002	-0.301	0.007	0.007	-0.098	1.309	-0.103
1.350	1.697	0.107	-0.154	0.019	0.007	-0.073	1.335	-0.052
1.375	1.644	0.168	-0.028	0.020	-0.005	-0.031	1.356	0.001
1.400	1.571	0.181	0.017	0.022	-0.002	0.002	1.380	0.050
1.425	1.485	0.168	0.021	0.015	0.004	0.001	1.345	0.069
1.450	1.410	0.158	0.028	0.016	0.007	-0.003	1.300	0.082
1.475	1.348	0.143	0.015	0.023	0.003	0.001	1.265	0.096
1.500	1.292	0.134	0.013	0.014	0.003	0.004	1.229	0.103
1.525	1.234	0.128	0.019	0.019	0.004	-0.009	1.195	0.114
1.550	1.187	0.119	0.015	0.012	-0.001	-0.002	1.163	0.115
1.575	1.133	0.110	0.022	0.009	-0.002	-0.003	1.133	0.122
1.600	1.096	0.100	0.015	0.013	-0.001	-0.009	1.105	0.125
1.625	1.070	0.095	0.017	0.011	-0.001	-0.005	1.081	0.126
1.650	1.032	0.085	0.015	0.009	0.002	-0.005	1.052	0.118
1.675	0.995	0.084	0.017	0.012	0.005	-0.003	1.030	0.122
1.700	0.974	0.074	0.006	0.006	0.001	-0.004	1.006	0.117

TABLE VII
(Continued)

R	g_{000}	g_{200}	g_{220}	g_{221}	g_{222}	g_{400}	G_{000}	G_{100}
1.725	0.945	0.068	0.011	0.004	0.005	-0.009	0.988	0.109
1.750	0.927	0.062	0.016	0.012	0.003	-0.007	0.971	0.104
1.775	0.908	0.060	0.005	0.009	-0.001	-0.008	0.953	0.092
1.800	0.897	0.049	0.008	0.006	0.003	-0.010	0.941	0.083
1.825	0.886	0.043	0.010	0.006	0.003	-0.012	0.926	0.071
1.850	0.875	0.040	0.018	0.004	0.002	-0.004	0.917	0.061
1.875	0.867	0.031	0.008	0.004	-0.001	-0.006	0.905	0.047
1.900	0.857	0.027	0.013	0.006	0.001	-0.009	0.902	0.037
1.925	0.861	0.022	0.015	0.003	-0.003	-0.009	0.898	0.031
1.950	0.862	0.013	0.011	0.004	-0.003	-0.009	0.897	0.020
1.975	0.863	0.009	0.016	0.003	-0.001	-0.004	0.900	0.012
2.000	0.864	0.003	0.018	0.003	0.003	-0.003	0.905	0.001
2.050	0.879	-0.008	0.018	0.004	-0.004	0.000	0.915	-0.015
2.100	0.897	-0.020	0.018	-0.004	-0.002	0.000	0.933	-0.026
2.150	0.917	-0.024	0.012	-0.003	-0.002	0.004	0.945	-0.033
2.200	0.953	-0.035	0.010	-0.004	0.004	0.003	0.967	-0.039
2.250	0.981	-0.033	0.005	-0.005	0.004	-0.001	0.983	-0.041
2.300	1.006	-0.033	-0.003	-0.003	-0.002	0.004	1.002	-0.040
2.350	1.021	-0.025	0.003	-0.001	0.000	0.000	1.014	-0.035
2.400	1.042	-0.022	-0.003	-0.002	-0.002	0.005	1.027	-0.031
2.450	1.055	-0.017	-0.006	-0.001	-0.005	0.003	1.035	-0.023
2.500	1.058	-0.014	-0.008	-0.004	-0.003	0.001	1.039	-0.016
2.550	1.063	-0.007	-0.003	-0.001	0.000	0.003	1.040	-0.009
2.600	1.057	0.000	-0.004	0.001	-0.001	-0.001	1.039	0.000
2.650	1.049	0.003	-0.007	0.003	0.000	0.003	1.037	0.005
2.700	1.039	0.007	-0.005	0.003	0.002	-0.002	1.030	0.010
2.750	1.035	0.010	-0.006	0.001	-0.004	0.000	1.025	0.012
2.800	1.018	0.010	-0.004	0.005	0.000	0.001	1.019	0.015
2.850	1.011	0.014	-0.003	0.003	-0.002	-0.004	1.011	0.015
2.900	1.003	0.010	0.004	0.001	-0.002	-0.003	0.999	0.024
2.950	0.995	0.007	-0.002	0.000	0.000	-0.002	0.992	0.052
3.000	0.989	0.009	0.003	0.001	0.000	-0.003	0.991	0.096

TABLE VII
(Continued)

R	g_{000}	g_{200}	g_{220}	g_{221}	g_{222}	g_{400}	G_{000}	G_{100}
			$L = 0.4$,	$\eta = 0.4189$				
0.975	0.006	-0.007	0.007	0.000	-0.010	0.007		
1.000	0.074	-0.080	0.087	-0.003	-0.051	0.075	1.511	-0.990
1.025	0.252	-0.264	0.276	-0.018	-0.044	0.227	1.492	-0.892
1.050	0.449	-0.447	0.444	-0.043	-0.019	0.339	1.483	-0.804
1.075	0.663	-0.615	0.564	-0.077	-0.009	0.387	1.459	-0.712
1.100	0.904	-0.764	0.615	-0.113	-0.008	0.369	1.448	-0.628
1.125	1.120	-0.833	0.540	-0.148	0.000	0.273	1.427	-0.545
1.150	1.352	-0.844	0.342	-0.172	0.005	0.166	1.419	-0.470
1.175	1.610	-0.779	-0.006	-0.179	0.003	0.111	1.411	-0.395
1.200	1.848	-0.654	-0.397	-0.168	0.007	0.122	1.394	-0.321
1.225	1.975	-0.492	-0.650	-0.136	0.010	0.077	1.389	-0.249
1.250	2.042	-0.312	-0.764	-0.092	0.008	-0.012	1.383	-0.185
1.275	2.038	-0.135	-0.734	-0.039	0.012	-0.094	1.380	-0.121
1.300	2.016	0.028	-0.597	-0.002	0.012	-0.153	1.384	-0.060
1.325	1.958	0.188	-0.399	0.033	0.004	-0.157	1.391	0.001
1.350	1.851	0.294	-0.178	0.046	0.009	-0.102	1.406	0.067
1.375	1.764	0.377	0.009	0.049	0.007	-0.026	1.421	0.134
1.400	1.608	0.357	0.076	0.045	0.006	-0.003	1.426	0.187
1.425	1.473	0.324	0.074	0.029	0.001	0.004	1.359	0.202
1.450	1.352	0.292	0.082	0.030	0.007	-0.001	1.282	0.201
1.475	1.261	0.262	0.067	0.034	0.001	-0.008	1.221	0.204
1.500	1.164	0.228	0.070	0.022	0.003	-0.010	1.152	0.203
1.525	1.085	0.195	0.049	0.027	0.001	-0.015	1.100	0.200
1.550	1.012	0.174	0.049	0.024	0.000	-0.016	1.054	0.194
1.575	0.967	0.160	0.044	0.018	0.005	-0.014	1.011	0.187
1.600	0.913	0.138	0.033	0.023	-0.004	-0.017	0.973	0.184
1.625	0.870	0.124	0.028	0.018	-0.002	-0.017	0.940	0.173
1.650	0.835	0.114	0.031	0.013	0.002	-0.018	0.910	0.161
1.675	0.803	0.098	0.033	0.015	-0.002	-0.014	0.886	0.153
1.700	0.781	0.081	0.032	0.013	0.002	-0.020	0.869	0.138

TABLE VII
(Continued)

R	g_{000}	g_{200}	g_{220}	g_{221}	g_{222}	g_{400}	G_{000}	G_{100}
1.725	0.760	0.071	0.029	0.010	0.000	-0.019	0.851	0.122
1.750	0.755	0.059	0.025	0.008	-0.002	-0.023	0.833	0.107
1.775	0.734	0.049	0.030	0.004	0.002	-0.015	0.827	0.085
1.800	0.738	0.043	0.030	0.007	-0.001	-0.015	0.818	0.068
1.825	0.730	0.032	0.020	0.004	-0.001	-0.018	0.812	0.049
1.850	0.729	0.017	0.023	0.005	0.001	-0.017	0.814	0.027
1.875	0.742	0.006	0.024	0.006	-0.001	-0.018	0.814	0.008
1.900	0.751	-0.002	0.023	0.008	-0.004	-0.012	0.821	-0.007
1.925	0.763	-0.014	0.027	0.001	-0.001	-0.013	0.833	-0.021
1.950	0.782	-0.028	0.027	0.002	-0.002	-0.009	0.849	-0.036
1.975	0.807	-0.034	0.025	0.003	-0.002	-0.007	0.869	-0.047
2.000	0.829	-0.042	0.032	-0.001	-0.002	-0.001	0.889	-0.060
2.050	0.877	-0.063	0.029	-0.003	-0.004	0.004	0.934	-0.078
2.100	0.940	-0.073	0.024	-0.008	-0.003	0.008	0.973	-0.086
2.150	1.001	-0.078	0.018	-0.003	-0.002	0.013	1.011	-0.086
2.200	1.055	-0.076	0.002	-0.009	0.000	0.014	1.042	-0.079
2.250	1.093	-0.066	-0.010	-0.010	0.005	0.015	1.063	-0.067
2.300	1.125	-0.046	-0.027	-0.007	0.003	0.011	1.081	-0.054
2.350	1.139	-0.034	-0.022	-0.005	-0.002	0.005	1.091	-0.035
2.400	1.136	-0.018	-0.020	-0.002	0.000	0.006	1.092	-0.017
2.450	1.129	0.001	-0.015	0.001	-0.002	0.009	1.085	0.000
2.500	1.111	0.014	-0.019	-0.001	0.000	0.003	1.074	0.016
2.550	1.086	0.025	-0.016	-0.001	0.000	0.002	1.058	0.026
2.600	1.061	0.030	-0.012	-0.001	0.001	-0.004	1.042	0.035
2.650	1.031	0.035	-0.005	0.003	-0.001	-0.001	1.021	0.039
2.700	1.010	0.036	-0.003	0.001	-0.003	-0.004	1.006	0.040
2.750	0.982	0.036	0.001	0.004	-0.002	-0.002	0.990	0.039
2.800	0.962	0.029	0.002	0.005	0.001	-0.008	0.976	0.032
2.850	0.949	0.023	0.004	0.002	-0.003	-0.005	0.968	0.027
2.900	0.944	0.015	0.005	-0.001	0.001	-0.006	0.955	0.026
2.950	0.938	0.008	0.010	0.000	0.003	-0.007	0.934	0.048
3.000	0.940	0.003	0.011	0.000	0.002	-0.003	0.901	0.086

TABLE VII
(Continued)

R	g_{000}	g_{200}	g_{220}	g_{221}	g_{222}	g_{400}	G_{000}	G_{100}
			L = 0.4,	η = 0.4712				
0.975	0.009	-0.010	0.011	0.000	-0.015	0.010		
1.000	0.109	-0.118	0.128	-0.004	-0.073	0.110	1.932	-1.251
1.025	0.343	-0.359	0.376	-0.025	-0.042	0.308	1.854	-1.088
1.050	0.587	-0.583	0.578	-0.059	-0.028	0.438	1.773	-0.936
1.075	0.826	-0.765	0.697	-0.099	-0.002	0.477	1.700	-0.801
1.100	1.076	-0.903	0.721	-0.141	0.005	0.426	1.642	-0.680
1.125	1.324	-0.972	0.610	-0.179	0.011	0.305	1.589	-0.567
1.150	1.584	-0.961	0.342	-0.206	0.017	0.174	1.536	-0.462
1.175	1.847	-0.840	-0.122	-0.212	0.011	0.115	1.496	-0.370
1.200	2.092	-0.653	-0.626	-0.199	0.019	0.140	1.455	-0.282
1.225	2.210	-0.457	-0.895	-0.146	0.024	0.086	1.428	-0.200
1.250	2.232	-0.246	-0.987	-0.083	0.011	-0.007	1.403	-0.129
1.275	2.197	-0.037	-0.905	-0.020	0.009	-0.123	1.389	-0.058
1.300	2.141	0.148	-0.704	0.028	0.011	-0.188	1.387	0.010
1.325	2.022	0.326	-0.435	0.061	0.012	-0.194	1.390	0.083
1.350	1.900	0.454	-0.142	0.084	0.002	-0.139	1.408	0.151
1.375	1.757	0.513	0.088	0.072	0.011	-0.047	1.423	0.221
1.400	1.566	0.481	0.172	0.064	0.002	0.005	1.424	0.282
1.425	1.403	0.415	0.150	0.053	0.006	-0.010	1.329	0.283
1.450	1.251	0.359	0.136	0.043	0.001	-0.011	1.233	0.275
1.475	1.133	0.309	0.105	0.040	0.008	-0.019	1.148	0.265
1.500	1.027	0.262	0.096	0.034	0.005	-0.021	1.075	0.254
1.525	0.949	0.223	0.075	0.031	0.002	-0.027	1.010	0.240
1.550	0.880	0.197	0.062	0.024	0.005	-0.028	0.955	0.221
1.575	0.819	0.169	0.061	0.026	0.002	-0.029	0.914	0.213
1.600	0.774	0.152	0.052	0.025	0.001	-0.026	0.877	0.198
1.625	0.729	0.122	0.050	0.016	0.001	-0.031	0.837	0.184
1.650	0.703	0.108	0.040	0.014	0.001	-0.029	0.814	0.168
1.675	0.680	0.088	0.037	0.007	0.001	-0.024	0.795	0.150
1.700	0.665	0.075	0.038	0.015	0.000	-0.030	0.779	0.133

TABLE VII
(Continued)

R	g_{000}	g_{200}	g_{220}	g_{221}	g_{222}	g_{400}	G_{000}	G_{100}
1.725	0.648	0.059	0.034	0.008	0.001	-0.024	0.771	0.112
1.750	0.641	0.044	0.033	0.006	-0.001	-0.024	0.763	0.091
1.775	0.646	0.028	0.028	0.003	-0.003	-0.025	0.762	0.064
1.800	0.650	0.018	0.032	0.005	-0.004	-0.022	0.761	0.038
1.825	0.661	0.005	0.035	0.004	-0.001	-0.021	0.770	0.009
1.850	0.678	-0.007	0.026	0.004	0.000	-0.019	0.777	-0.015
1.875	0.694	-0.022	0.035	0.003	0.000	-0.014	0.796	-0.034
1.900	0.725	-0.038	0.040	-0.003	-0.002	-0.011	0.818	-0.053
1.925	0.754	-0.051	0.038	0.002	-0.006	-0.010	0.841	-0.070
1.950	0.790	-0.065	0.037	-0.002	-0.006	-0.001	0.868	-0.085
1.975	0.825	-0.075	0.035	-0.005	-0.002	-0.002	0.893	-0.097
2.000	0.869	-0.086	0.036	-0.004	-0.003	0.005	0.926	-0.108
2.050	0.953	-0.105	0.029	-0.006	-0.006	0.017	0.987	-0.121
2.100	1.029	-0.109	0.023	-0.006	-0.003	0.020	1.037	-0.119
2.150	1.096	-0.103	0.005	-0.009	-0.008	0.027	1.076	-0.105
2.200	1.155	-0.088	-0.022	-0.012	0.000	0.021	1.103	-0.082
2.250	1.187	-0.061	-0.030	-0.012	0.000	0.019	1.120	-0.059
2.300	1.199	-0.032	-0.042	-0.007	0.000	0.012	1.128	-0.036
2.350	1.201	-0.008	-0.030	-0.006	0.000	0.008	1.125	-0.010
2.400	1.182	0.014	-0.026	0.001	0.004	0.011	1.114	0.013
2.450	1.142	0.027	-0.019	-0.001	0.001	0.006	1.094	0.032
2.500	1.106	0.042	-0.021	0.002	-0.001	0.000	1.066	0.047
2.550	1.062	0.048	-0.014	0.004	0.001	0.000	1.035	0.057
2.600	1.016	0.051	-0.010	0.002	-0.001	-0.007	1.008	0.060
2.650	0.982	0.055	-0.003	0.001	-0.001	-0.012	0.981	0.061
2.700	0.944	0.049	-0.001	0.003	-0.003	-0.013	0.961	0.055
2.750	0.918	0.043	0.008	0.003	-0.001	-0.010	0.944	0.046
2.800	0.900	0.031	0.012	0.004	-0.003	-0.007	0.932	0.031
2.850	0.896	0.020	0.014	0.002	-0.002	-0.009	0.932	0.018
2.900	0.901	0.010	0.014	0.003	-0.002	-0.007	0.932	0.011
2.950	0.907	-0.005	0.016	0.001	-0.001	-0.005	0.921	0.027
3.000	0.927	-0.015	0.015	-0.001	-0.003	-0.005	0.892	0.064

TABLE VII
(Continued)

R	g_{000}	g_{200}	g_{220}	g_{221}	g_{222}	g_{400}	G_{000}	G_{100}
			L = 0.6,	η = 0.2094				
0.950	0.006	−0.007	0.007	0.000	−0.010	0.006		
0.975	0.022	−0.024	0.026	−0.001	−0.030	0.022		
1.000	0.057	−0.060	0.063	−0.003	−0.049	0.052	0.789	−0.469
1.025	0.114	−0.116	0.118	−0.012	−0.044	0.093	0.805	−0.455
1.050	0.180	−0.177	0.175	−0.023	−0.036	0.130	0.829	−0.443
1.075	0.252	−0.237	0.223	−0.038	−0.038	0.154	0.842	−0.427
1.100	0.340	−0.304	0.269	−0.056	−0.034	0.171	0.860	−0.412
1.125	0.427	−0.360	0.295	−0.073	−0.029	0.170	0.873	−0.394
1.150	0.515	−0.404	0.297	−0.093	−0.023	0.152	0.889	−0.375
1.175	0.604	−0.436	0.277	−0.107	−0.028	0.127	0.910	−0.360
1.200	0.697	−0.455	0.230	−0.124	−0.023	0.095	0.923	−0.339
1.225	0.807	−0.464	0.150	−0.138	−0.009	0.071	0.939	−0.322
1.250	0.911	−0.458	0.056	−0.139	−0.007	0.062	0.952	−0.303
1.275	1.006	−0.426	−0.074	−0.136	−0.010	0.063	0.966	−0.276
1.300	1.083	−0.392	−0.167	−0.123	−0.013	0.056	0.981	−0.259
1.325	1.165	−0.355	−0.246	−0.106	−0.009	0.037	0.985	−0.238
1.350	1.208	−0.307	−0.288	−0.093	−0.005	0.017	1.007	−0.215
1.375	1.251	−0.250	−0.324	−0.076	0.006	−0.009	1.020	−0.196
1.400	1.300	−0.204	−0.331	−0.055	0.000	−0.031	1.033	−0.170
1.425	1.322	−0.152	−0.312	−0.040	0.001	−0.053	1.049	−0.150
1.450	1.330	−0.089	−0.281	−0.015	0.005	−0.068	1.061	−0.126
1.475	1.337	−0.043	−0.225	−0.005	0.000	−0.068	1.081	−0.104
1.500	1.340	0.007	−0.176	0.007	0.000	−0.063	1.095	−0.084
1.525	1.336	0.043	−0.108	0.008	−0.004	−0.049	1.107	−0.056
1.550	1.316	0.071	−0.045	0.016	0.003	−0.033	1.124	−0.034
1.575	1.298	0.087	−0.012	0.017	0.008	−0.008	1.137	−0.009
1.600	1.268	0.098	0.000	0.014	0.009	−0.004	1.149	0.014
1.625	1.235	0.088	0.007	0.010	0.000	0.006	1.143	0.019
1.650	1.215	0.094	0.010	0.012	0.001	0.002	1.126	0.028
1.675	1.191	0.089	0.008	0.008	0.007	−0.001	1.115	0.027
1.700	1.155	0.082	0.010	0.012	0.006	0.000	1.100	0.035

TABLE VII
(Continued)

R	g_{000}	g_{200}	g_{220}	g_{221}	g_{222}	g_{400}	G_{000}	G_{100}
1.725	1.137	0.077	0.007	0.010	0.000	-0.006	1.088	0.037
1.750	1.110	0.069	0.014	0.013	0.000	0.000	1.078	0.041
1.775	1.087	0.067	0.008	0.008	-0.004	-0.002	1.067	0.044
1.800	1.082	0.070	0.012	0.012	-0.006	0.001	1.060	0.046
1.825	1.058	0.062	0.005	0.013	0.000	-0.004	1.049	0.047
1.850	1.044	0.061	0.013	0.009	0.005	-0.002	1.039	0.050
1.875	1.032	0.055	0.012	0.010	0.003	-0.002	1.031	0.049
1.900	1.020	0.052	0.014	0.003	0.001	-0.003	1.022	0.050
1.925	1.011	0.050	0.012	0.008	0.003	-0.003	1.016	0.050
1.950	0.997	0.046	0.012	0.005	0.003	0.000	1.012	0.049
1.975	0.982	0.036	0.007	0.006	-0.001	-0.001	1.009	0.047
2.000	0.979	0.037	0.012	0.009	-0.001	-0.004	1.004	0.044
2.050	0.967	0.030	0.009	0.009	0.001	-0.001	0.995	0.040
2.100	0.956	0.019	0.011	0.004	-0.001	-0.005	0.992	0.035
2.150	0.956	0.012	0.015	0.000	0.001	0.004	0.986	0.028
2.200	0.958	0.011	0.015	0.004	-0.004	-0.002	0.986	0.021
2.250	0.952	0.003	0.017	0.004	-0.001	0.006	0.983	0.011
2.300	0.961	-0.002	0.008	0.004	-0.001	-0.004	0.981	0.005
2.350	0.963	-0.007	0.006	0.001	-0.003	0.001	0.981	-0.001
2.400	0.968	-0.008	0.010	-0.002	-0.002	0.000	0.985	-0.003
2.450	0.980	-0.012	0.002	0.001	-0.001	0.002	0.989	-0.008
2.500	0.986	-0.012	0.003	-0.002	-0.001	0.000	0.990	-0.011
2.550	0.992	-0.012	0.004	-0.001	-0.001	0.001	0.995	-0.012
2.600	0.995	-0.009	-0.002	-0.001	0.002	0.002	0.995	-0.010
2.650	1.006	-0.014	0.002	0.001	-0.002	-0.001	0.999	-0.011
2.700	1.003	-0.009	0.002	-0.004	-0.003	0.004	1.000	-0.005
2.750	1.007	-0.008	-0.002	-0.002	-0.002	-0.002	0.992	0.012
2.800	1.012	-0.009	-0.004	0.000	0.002	0.005	0.974	0.038
2.850	1.017	-0.006	-0.001	-0.001	-0.001	-0.001	0.950	0.071
2.900	1.018	-0.003	-0.003	0.000	0.001	0.000	0.919	0.109
2.950	1.016	-0.002	-0.001	-0.001	0.001	-0.001	0.877	0.146
3.000	1.017	-0.003	-0.003	0.000	0.000	0.001	0.000	0.000

TABLE VII
(Continued)

R	g_{000}	g_{200}	g_{220}	g_{221}	g_{222}	g_{400}	G_{000}	G_{100}
			L = 0.6,	η = 0.3142				
0.950	0.009	-0.010	0.011	0.000	-0.015	0.010		
0.975	0.038	-0.041	0.044	-0.001	-0.053	0.038		
1.000	0.094	-0.099	0.104	-0.006	-0.076	0.085	1.168	-0.673
1.025	0.189	-0.192	0.195	-0.021	-0.064	0.152	1.164	-0.631
1.050	0.293	-0.287	0.281	-0.041	-0.051	0.206	1.153	-0.593
1.075	0.399	-0.373	0.348	-0.065	-0.037	0.237	1.155	-0.554
1.100	0.511	-0.455	0.400	-0.088	-0.038	0.252	1.144	-0.513
1.125	0.617	-0.515	0.416	-0.113	-0.026	0.234	1.139	-0.475
1.150	0.729	-0.566	0.410	-0.138	-0.015	0.206	1.134	-0.438
1.175	0.842	-0.597	0.365	-0.161	-0.010	0.159	1.136	-0.410
1.200	0.957	-0.609	0.285	-0.177	-0.002	0.112	1.125	-0.370
1.225	1.059	-0.590	0.157	-0.183	-0.004	0.077	1.117	-0.334
1.250	1.179	-0.556	0.001	-0.191	-0.002	0.065	1.118	-0.300
1.275	1.294	-0.499	-0.190	-0.175	0.004	0.079	1.120	-0.271
1.300	1.369	-0.441	-0.318	-0.155	0.000	0.070	1.113	-0.236
1.325	1.428	-0.370	-0.417	-0.137	0.000	0.047	1.115	-0.205
1.350	1.477	-0.303	-0.471	-0.112	0.000	0.010	1.113	-0.176
1.375	1.504	-0.224	-0.505	-0.077	-0.005	-0.017	1.115	-0.148
1.400	1.521	-0.152	-0.485	-0.055	0.015	-0.055	1.118	-0.116
1.425	1.520	-0.076	-0.444	-0.024	0.006	-0.085	1.123	-0.089
1.450	1.508	-0.009	-0.386	-0.006	0.008	-0.095	1.127	-0.060
1.475	1.491	0.060	-0.301	0.012	0.010	-0.092	1.131	-0.033
1.500	1.467	0.117	-0.217	0.026	0.007	-0.088	1.134	-0.007
1.525	1.428	0.164	-0.121	0.033	0.004	-0.064	1.149	0.021
1.550	1.383	0.194	-0.036	0.039	0.008	-0.039	1.157	0.051
1.575	1.346	0.213	0.019	0.035	0.005	-0.008	1.172	0.075
1.600	1.286	0.212	0.050	0.032	0.003	0.004	1.175	0.100
1.625	1.238	0.193	0.042	0.032	0.004	-0.006	1.151	0.105
1.650	1.190	0.184	0.044	0.036	0.000	-0.002	1.123	0.107
1.675	1.135	0.169	0.039	0.031	0.001	-0.006	1.091	0.101
1.700	1.096	0.155	0.039	0.030	0.001	-0.007	1.069	0.103

TABLE VII
(Continued)

R	g_{000}	g_{200}	g_{220}	g_{221}	g_{222}	g_{400}	G_{000}	G_{100}
1.725	1.061	0.142	0.032	0.028	0.000	-0.008	1.049	0.100
1.750	1.032	0.133	0.034	0.023	0.002	-0.009	1.032	0.097
1.775	1.006	0.122	0.032	0.020	-0.001	-0.011	1.014	0.095
1.800	0.980	0.110	0.031	0.025	0.004	-0.010	0.998	0.091
1.825	0.957	0.103	0.030	0.015	0.002	-0.007	0.988	0.088
1.850	0.936	0.089	0.028	0.022	0.001	-0.011	0.972	0.085
1.875	0.920	0.078	0.028	0.013	0.002	-0.009	0.964	0.077
1.900	0.905	0.071	0.027	0.012	0.003	-0.009	0.957	0.073
1.925	0.896	0.060	0.033	0.011	-0.003	-0.008	0.952	0.065
1.950	0.885	0.050	0.035	0.011	0.002	-0.006	0.949	0.060
1.975	0.878	0.040	0.029	0.010	-0.002	-0.004	0.948	0.052
2.000	0.883	0.033	0.030	0.007	0.003	-0.004	0.949	0.045
2.050	0.876	0.016	0.039	0.008	0.000	-0.001	0.954	0.029
2.100	0.882	0.000	0.034	0.004	0.000	0.002	0.957	0.016
2.150	0.892	-0.012	0.030	-0.001	0.001	0.004	0.962	0.005
2.200	0.915	-0.023	0.028	-0.001	-0.001	0.007	0.968	-0.009
2.250	0.929	-0.036	0.022	-0.004	-0.002	0.005	0.974	-0.019
2.300	0.957	-0.040	0.013	-0.005	0.000	0.002	0.979	-0.024
2.350	0.980	-0.041	0.005	-0.004	0.001	0.002	0.989	-0.028
2.400	1.002	-0.039	-0.004	-0.002	-0.001	0.003	0.998	-0.031
2.450	1.012	-0.036	-0.004	0.000	0.004	0.004	1.001	-0.031
2.500	1.023	-0.028	-0.005	-0.001	0.000	0.000	1.009	-0.027
2.550	1.030	-0.019	-0.010	-0.004	0.002	0.004	1.013	-0.023
2.600	1.035	-0.017	-0.011	-0.002	0.001	0.005	1.019	-0.017
2.650	1.044	-0.009	-0.008	-0.002	-0.002	0.001	1.020	-0.014
2.700	1.039	-0.006	-0.015	-0.001	0.004	0.002	1.018	-0.006
2.750	1.038	-0.002	-0.012	-0.001	0.002	0.002	1.006	0.016
2.800	1.036	0.006	-0.010	-0.003	0.000	-0.001	0.985	0.045
2.850	1.028	0.006	-0.010	-0.002	0.001	-0.002	0.959	0.080
2.900	1.028	0.007	-0.006	-0.001	-0.001	-0.002	0.923	0.117
2.950	1.020	0.010	-0.002	0.002	0.001	0.000	0.880	0.155
3.000	1.012	0.012	-0.003	0.004	0.001	-0.002	0.000	0.000

TABLE VII
(Continued)

R	g_{000}	g_{200}	g_{220}	g_{221}	g_{222}	g_{400}	G_{000}	G_{100}
			L = 0.6,	η = 0.4189				
0.925	0.003	-0.003	0.004	0.000	-0.005	0.003		
0.950	0.024	-0.026	0.029	0.000	-0.040	0.026		
0.975	0.078	-0.084	0.091	-0.002	-0.107	0.078		
1.000	0.195	-0.205	0.215	-0.013	-0.154	0.177	1.847	-1.003
1.025	0.354	-0.359	0.365	-0.040	-0.106	0.284	1.759	-0.895
1.050	0.528	-0.514	0.502	-0.079	-0.064	0.365	1.665	-0.789
1.075	0.661	-0.615	0.572	-0.112	-0.033	0.385	1.585	-0.697
1.100	0.790	-0.696	0.606	-0.147	-0.013	0.372	1.520	-0.616
1.125	0.912	-0.749	0.592	-0.185	0.005	0.320	1.454	-0.542
1.150	1.020	-0.774	0.539	-0.206	-0.003	0.254	1.395	-0.474
1.175	1.130	-0.774	0.437	-0.235	0.006	0.173	1.340	-0.409
1.200	1.235	-0.746	0.290	-0.247	.0.004	0.100	1.293	-0.350
1.225	1.349	-0.688	0.077	-0.252	0.001	0.050	1.253	-0.299
1.250	1.477	-0.609	-0.182	-0.250	0.006	0.064	1.220	-0.251
1.275	1.578	-0.502	-0.448	-0.222	0.000	0.098	1.188	-0.207
1.300	1.648	-0.389	-0.634	-0.193	0.010	0.094	1.156	-0.162
1.325	1.669	-0.295	-0.724	-0.160	0.000	0.055	1.138	-0.124
1.350	1.687	-0.199	-0.769	-0.105	0.010	0.017	1.117	-0.090
1.375	1.674	-0.099	-0.757	-0.065	0.003	-0.035	1.101	-0.054
1.400	1.650	-0.005	-0.700	-0.026	0.005	-0.089	1.094	-0.024
1.425	1.615	0.092	-0.606	0.016	0.010	-0.136	1.086	0.005
1.450	1.570	0.174	-0.484	0.047	0.014	-0.152	1.087	0.036
1.475	1.514	0.250	-0.348	0.061	0.011	-0.153	1.089	0.066
1.500	1.469	0.314	-0.200	0.082	0.007	-0.137	1.092	0.093
1.525	1.401	0.354	-0.062	0.088	0.003	-0.095	1.105	0.123
1.550	1.328	0.381	0.053	0.081	0.008	-0.054	1.114	0.152
1.575	1.256	0.387	0.137	0.080	0.006	-0.014	1.127	0.179
1.600	1.173	0.357	0.151	0.073	0.005	-0.006	1.129	0.202
1.625	1.099	0.315	0.143	0.058	0.003	-0.007	1.093	0.192
1.650	1.026	0.278	0.129	0.058	0.005	-0.011	1.046	0.179
1.675	0.980	0.248	0.117	0.051	-0.002	-0.010	1.006	0.166
1.700	0.929	0.219	0.106	0.046	0.004	-0.019	0.973	0.151

TABLE VII
(Continued)

R	g_{000}	g_{200}	g_{220}	g_{221}	g_{222}	g_{400}	G_{000}	G_{100}
1.725	0.884	0.189	0.094	0.039	-0.003	-0.016	0.950	0.138
1.750	0.861	0.163	0.088	0.035	0.004	-0.022	0.926	0.126
1.775	0.829	0.143	0.089	0.030	0.002	-0.021	0.907	0.112
1.800	0.806	0.124	0.080	0.028	0.002	-0.017	0.899	0.102
1.825	0.789	0.102	0.080	0.020	0.002	-0.018	0.889	0.090
1.850	0.778	0.082	0.072	0.023	0.000	-0.016	0.887	0.076
1.875	0.769	0.065	0.068	0.018	-0.002	-0.016	0.884	0.061
1.900	0.766	0.045	0.071	0.018	0.000	-0.008	0.887	0.051
1.925	0.774	0.030	0.070	0.014	-0.003	-0.009	0.896	0.037
1.950	0.776	0.010	0.068	0.011	0.001	-0.004	0.906	0.023
1.975	0.782	-0.009	0.068	0.006	-0.002	0.002	0.915	0.010
2.000	0.797	-0.018	0.077	0.005	-0.001	0.002	0.931	-0.006
2.050	0.829	-0.056	0.070	0.000	-0.003	0.011	0.963	-0.025
2.100	0.877	-0.078	0.066	-0.003	-0.004	0.013	0.982	-0.038
2.150	0.921	-0.096	0.054	-0.009	-0.006	0.017	1.000	-0.051
2.200	0.968	-0.103	0.029	-0.010	-0.002	0.014	1.008	-0.054
2.250	1.006	-0.098	0.008	-0.015	-0.003	0.014	1.016	-0.058
2.300	1.043	-0.086	-0.014	-0.013	0.001	0.011	1.023	-0.055
2.350	1.071	-0.067	-0.032	-0.013	-0.002	0.009	1.027	-0.048
2.400	1.085	-0.047	-0.044	-0.009	0.003	0.007	1.032	-0.037
2.450	1.094	-0.031	-0.044	-0.005	0.001	0.002	1.035	-0.029
2.500	1.094	-0.011	-0.042	-0.002	-0.001	0.003	1.036	-0.018
2.550	1.085	0.005	-0.030	0.000	0.001	-0.001	1.036	-0.006
2.600	1.071	0.017	-0.021	0.002	0.003	0.000	1.032	0.002
2.650	1.064	0.022	-0.018	0.004	-0.001	0.001	1.026	0.011
2.700	1.046	0.030	-0.012	0.004	0.000	-0.003	1.016	0.019
2.750	1.030	0.032	-0.012	0.003	-0.001	-0.001	0.996	0.040
2.800	1.018	0.032	-0.009	0.006	0.000	-0.004	0.971	0.066
2.850	1.000	0.030	-0.003	0.003	0.001	-0.004	0.944	0.097
2.900	0.987	0.032	0.001	0.005	-0.001	-0.004	0.904	0.130
2.950	0.976	0.022	0.005	0.004	0.000	-0.008	0.863	0.163
3.000	0.970	0.019	0.008	0.004	0.002	-0.004	0.000	0.000

TABLE VII
(Continued)

R	g_{000}	g_{200}	g_{220}	g_{221}	g_{222}	g_{400}	G_{000}	G_{100}
			L = 0.6,	η = 0.4712				
0.925	0.004	-0.004	0.005	0.000	-0.007	0.004		
0.950	0.035	-0.039	0.042	0.000	-0.058	0.037		
0.975	0.111	-0.120	0.130	-0.002	-0.152	0.111		
1.000	0.265	-0.277	0.291	-0.019	-0.198	0.238	2.364	-1.256
1.025	0.490	-0.494	0.501	-0.060	-0.114	0.386	2.183	-1.085
1.050	0.672	-0.652	0.634	-0.105	-0.053	0.458	2.012	-0.926
1.075	0.831	-0.768	0.709	-0.150	-0.017	0.470	1.855	-0.779
1.100	0.950	-0.827	0.710	-0.189	0.012	0.424	1.713	-0.660
1.125	1.063	-0.862	0.671	-0.224	0.020	0.352	1.596	-0.555
1.150	1.161	-0.860	0.572	-0.255	0.022	0.251	1.498	-0.470
1.175	1.255	-0.828	0.424	-0.275	0.005	0.148	1.399	-0.386
1.200	1.376	-0.782	0.222	-0.293	0.011	0.062	1.332	-0.317
1.225	1.497	-0.702	-0.037	-0.296	0.010	0.019	1.263	-0.255
1.250	1.628	-0.578	-0.389	-0.288	0.003	0.054	1.209	-0.201
1.275	1.743	-0.455	-0.692	-0.256	0.007	0.110	1.163	-0.152
1.300	1.786	-0.329	-0.880	-0.204	0.002	0.109	1.121	-0.106
1.325	1.789	-0.213	-0.961	-0.156	0.007	0.072	1.089	-0.064
1.350	1.766	-0.101	-0.964	-0.099	0.004	0.007	1.069	-0.030
1.375	1.724	0.003	-0.907	-0.036	0.007	-0.062	1.051	0.003
1.400	1.668	0.100	-0.791	0.018	0.013	-0.132	1.033	0.033
1.425	1.613	0.198	-0.665	0.055	0.010	-0.181	1.034	0.064
1.450	1.554	0.284	-0.500	0.092	0.014	-0.207	1.032	0.094
1.475	1.486	0.360	-0.311	0.107	0.012	-0.205	1.042	0.124
1.500	1.419	0.430	-0.135	0.118	0.010	-0.172	1.055	0.154
1.525	1.342	0.471	0.035	0.117	0.011	-0.114	1.068	0.184
1.550	1.260	0.489	0.170	0.113	0.006	-0.062	1.085	0.212
1.575	1.169	0.470	0.243	0.098	0.005	-0.012	1.098	0.239
1.600	1.073	0.420	0.250	0.084	0.008	0.004	1.100	0.260
1.625	0.990	0.364	0.218	0.076	0.004	-0.008	1.045	0.236
1.650	0.910	0.307	0.181	0.062	0.007	-0.006	0.991	0.211
1.675	0.856	0.264	0.163	0.053	0.005	-0.018	0.948	0.187
1.700	0.805	0.225	0.142	0.046	0.004	-0.014	0.912	0.164

TABLE VII
(Continued)

R	g_{000}	g_{200}	g_{220}	g_{221}	g_{222}	g_{400}	G_{000}	G_{100}
1.725	0.763	0.192	0.132	0.040	0.000	-0.020	0.885	0.144
1.750	0.734	0.157	0.116	0.032	-0.001	-0.021	0.865	0.122
1.775	0.714	0.131	0.110	0.030	-0.001	-0.019	0.853	0.102
1.800	0.694	0.101	0.099	0.024	0.000	-0.020	0.847	0.081
1.825	0.690	0.077	0.095	0.019	0.001	-0.019	0.850	0.062
1.850	0.682	0.050	0.086	0.015	-0.002	-0.015	0.853	0.044
1.875	0.691	0.031	0.091	0.012	-0.001	-0.008	0.860	0.028
1.900	0.701	0.005	0.090	0.011	-0.002	-0.006	0.871	0.008
1.925	0.717	-0.015	0.090	0.006	-0.006	0.001	0.890	-0.005
1.950	0.740	-0.038	0.087	0.002	-0.007	0.007	0.911	-0.020
1.975	0.764	-0.058	0.088	0.000	-0.004	0.008	0.933	-0.035
2.000	0.797	-0.081	0.098	-0.002	-0.004	0.015	0.960	-0.052
2.050	0.862	-0.117	0.086	-0.008	-0.006	0.025	1.004	-0.070
2.100	0.929	-0.139	0.076	-0.017	-0.007	0.026	1.032	-0.076
2.150	0.991	-0.148	0.048	-0.018	-0.005	0.028	1.042	-0.078
2.200	1.048	-0.135	0.008	-0.019	-0.003	0.021	1.041	-0.076
2.250	1.087	-0.116	-0.037	-0.018	-0.003	0.014	1.044	-0.067
2.300	1.120	-0.087	-0.063	-0.018	-0.002	0.010	1.043	-0.054
2.350	1.138	-0.050	-0.086	-0.013	-0.003	0.003	1.042	-0.040
2.400	1.136	-0.020	-0.086	-0.005	-0.003	0.000	1.041	-0.024
2.450	1.128	0.006	-0.076	-0.001	-0.001	-0.001	1.040	-0.009
2.500	1.111	0.029	-0.050	0.001	-0.002	-0.002	1.037	0.005
2.550	1.084	0.042	-0.034	0.004	0.002	-0.008	1.034	0.017
2.600	1.062	0.048	-0.018	0.004	0.000	-0.006	1.025	0.027
2.650	1.034	0.051	-0.004	0.002	0.002	-0.003	1.015	0.032
2.700	1.012	0.049	-0.004	0.007	0.000	-0.007	0.996	0.039
2.750	0.992	0.050	-0.003	0.004	0.001	-0.008	0.977	0.053
2.800	0.968	0.042	0.000	0.007	0.001	-0.007	0.951	0.074
2.850	0.958	0.038	0.005	0.009	0.002	-0.007	0.922	0.100
2.900	0.947	0.027	0.008	0.003	0.000	-0.005	0.886	0.128
2.950	0.943	0.019	0.016	0.005	0.000	-0.006	0.000	0.000
3.000	0.943	0.008	0.022	0.002	0.001	-0.002	0.000	0.000

TABLE VIII

The fluid of hard homonuclear diatomics (L = 0.6, η = 0.4691): radial slices through g(1,2) at specific orientations

R	parallel	crossed	T-shaped
0.925		17.7	
0.965		13.4	
1.005	7.43	9.16	
1.045	6.99	6.12	
1.085	6.59	4.47	
1.125	4.66	3.31	
1.165	3.25	2.45	
1.205	2.53	1.94	
1.245	1.80	1.28	
1.265	1.53	1.15	7.96
1.305	1.25	0.98	5.53
1.345	1.00	0.75	4.17
1.385	0.79	0.61	3.23
1.425	0.72	0.58	2.32
1.465	0.56	0.54	1.92
1.505	0.47	0.46	1.52
1.545	0.49	0.37	1.25
1.585	0.44	0.38	1.02
1.625	0.48	0.38	0.79
1.665	0.44	0.40	0.74
1.705	0.43	0.38	0.70
1.805	0.53	0.50	0.53
1.905	0.81	0.77	0.48
2.005	1.12	1.25	0.52
2.105	1.35	1.40	0.64
2.205	1.33	1.36	0.90
2.305	1.18	1.16	1.15
2.505	1.00	0.97	1.14
2.705	0.86	0.86	0.97
2.995	0.95	0.96	0.84

TABLE IX

Fluids of hard homonuclear diatomics (L=0.6): radial slices through the background correlation function $y(1,2)$ at specific orientations. (Numbers in parentheses denote the error of last digits)

R	parallel	crossed	T-shaped	end-to-end
		$\eta = 0.1877$		
0.0	13.26	7.76(1)	7.76(1)	13.26
0.1	10.86(6)	7.46(2)	7.66(2)	11.34(3)
0.2	8.92(4)	6.79(3)	7.32(2)	9.80(8)
0.3	7.34(4)	5.98(5)	6.72(2)	8.52(4)
0.4	6.08(3)	5.18(4)	5.90(2)	7.42(12)
0.5	5.04(3)	4.44(2)	5.15(3)	6.56(26)
0.6	4.20(3)	3.77(4)	4.50(3)	5.85(5)
0.7	3.52(3)	3.21(5)	3.64(3)	5.11(24)
0.8	2.97(5)	2.75(5)	3.45(4)	4.43(33)
0.9	2.54(5)	2.36(4)	3.02(3)	3.87(26)
1.0	2.17(4)	2.05(4)	2.64(3)	3.39(12)
1.1	1.88(6)	1.78(4)	2.32(3)	2.97(5)
1.2	1.64(5)	1.58(4)	2.04(2)	2.63(3)
1.3	1.45(5)	1.40(5)	1.82(2)	2.32(7)
1.4	1.32(5)	1.26(6)	1.62(1)	2.06(3)
1.5	1.18(5)	1.15(5)	1.46(1)	1.85(10)
1.6	1.09(4)	1.07(4)	1.32(1)	1.64(12)
		$\eta = 0.2815$		
0.0	157.1	52.19(6)	52.19(6)	157.1
0.1	104.2(11)	48.13(16)	50.57(6)	115.0(14)
0.2	68.12(11)	39.41(14)	46.04(8)	85.1(15)
0.3	46.09(7)	30.06(12)	38.51(5)	63.7(20)
0.4	30.99(10)	21.97(14)	29.53(7)	48.5(20)
0.5	20.89(7)	15.84(16)	22.24(8)	37.4(6)
0.6	14.17(4)	11.31(10)	16.80(8)	29.43(12)
0.7	9.82(4)	8.09(5)	12.80(7)	21.93(6)

TABLE IX
(Continued)

R	parallel	crossed	T-shaped	end-to-end
		η = 0.2815		
0.8	6.90(5)	5.87(5)	9.69(5)	16.49(10)
0.9	4.97(8)	4.30(9)	7.30(5)	12.31(13)
1.0	3.61(8)	3.18(9)	5.53(5)	9.27(41)
1.1	2.68(5)	2.41(7)	4.18(4)	7.02(45)
1.2	2.02(6)	1.87(4)	3.21(4)	5.37(30)
1.3	1.56(3)	1.48(4)	2.51(4)	4.16(7)
1.4	1.26(3)	1.20(3)	1.97(3)	3.25(10)
1.5	1.07(3)	1.02(3)	1.61(3)	2.58(9)
1.6	0.93(4)	0.88(1)	1.33(3)	2.01(5)
		η = 0.3753		
0.0	10073.0	1109.0(100)	1109.0(100)	10073.0
0.1	4474.0(90)	950.0(50)	1052.0(20)	5522.0(310)
0.2	1990.0(80)	637.0(30)	881.0(20)	3110.0(390)
0.3	890.0(40)	369.0(20)	631.0(20)	1784.0(580)
0.4	403.0(30)	200.0(10)	379.0(20)	1054.0(250)
0.5	186.0(20)	104.0(20)	222.0(10)	649.0(100)
0.6	87.5(10)	52.9(12)	132.0(10)	413.0(150)
0.7	42.5(8)	27.6(7)	78.7(8)	237.0(130)
0.8	21.1(4)	14.8(3)	46.9(7)	136.0(110)
0.9	11.1(3)	8.3(2)	27.7(5)	79.0(100)
1.0	6.22(30)	4.7(2)	16.2(4)	47.0(50)
1.1	3.75(27)	2.9(3)	9.47(24)	27.3(25)
1.2	2.29(18)	1.80(35)	5.76(15)	16.8(13)
1.3	1.44(25)	1.13(28)	3.69(15)	10.7(13)
1.4	1.03(14)	0.96(20)	2.39(14)	7.10(99)
1.5	0.68(4)	0.76(20)	1.69(10)	4.53(90)
1.6	0.55(5)	0.73(10)	1.23(8)	2.97(32)

a series of densities and, in addition to the average site–site c.f., calculated also the spherical harmonic expansion coefficients $G^{\alpha\beta}_{100}$. Accuracy of these data ($N = 294$, $N_c = (1{\cdot}5-2{\cdot}5) \cdot 10^6$, $N_c/N_a = 588$), assessed both by means of the standard statistical methods and consistency checks, is 2 per cent for G_{AA} and G_{AB}, and about 5 per cent for G_{BB}. To enable one to study the effect of density on structural properties we list in Tables X and XI the data on the two above mentioned models. The effect of asymmetry may be studied using the data on other three models with the same $L = 0{\cdot}75$ and at the same packing fraction but with different diameters σ_B; these data (taken also from the paper by Streett and Tildesley[52]) are listed in Table XI as well.

Both in Table X and Table XI the covered site–site separations are in some cases relatively small; we remind in passing that at larger separations the functions $G_{\alpha\beta}$ may be calculated quite accurately using the RISM equation[32]. The nonequidistant mesh is used in order to cover more densily the vicinity of the cusps which occur at $L + (1 + \sigma_B)/2$ for G_{AA} and G_{BB}, and at separations $L + 1$ and $L + \sigma_B$ for G_{AB}.

Symmetric Triatomics

Linear symmetric triatomics models have been considered by Boublík[6], Streett and Tildesley[53], and Nezbeda et al.[39]. Boublík considered one model ($L = 0{\cdot}5$, $\sigma_B = 1$) at one density and his simulations aimed primarily at obtaining the equation of state. Streett and Tildesley obtained $G_{\alpha\beta}$ and coefficients g_{klm} for three different models $[(L, \sigma_B) = (0{\cdot}37375, 0{\cdot}8333), (0{\cdot}4485, 1{\cdot}0), (0{\cdot}5233, 1{\cdot}1669)]$, each also at one density only; accuracy of these data is estimated to be about 5 per cent at best. Nezbeda et al. investigated systematically one model ($L = 0{\cdot}8$, $\sigma_B = 1{\cdot}0$) at four densities. Besides the average site–site c.f. $G_{\alpha\beta}$ (G_{CC} exhibits a cusp at $1 + L/2$, for G_{BB} the cusps occur at $(1 + L^2/2)^{1/2}$ and $L + 1$, and for G_{CB} at $(1 + L^2/2)^{1/2}$ and $1 + L/2$) they also computed the site-site spherical harmonic expansion cofficients $G^{\alpha\beta}_{100}$. The latter data ($N = 192, /N_c = (1{\cdot}5-2{\cdot}5) \cdot 10^6$, $N_c/N_a = 576$) are summarized in Table XII. Their accuracy is about 2 per cent.

In addition to a model of only mild nonsphericity ($L = 0{\cdot}5$, $\sigma_B = 1$, $\omega = 90°$) simulated by Boublík[6] to obtain the equation of state at one density, we are aware of only one simulations on a nonlinear model of symmetric triatomics ($L = 0{\cdot}8$, $\sigma_B = 0{\cdot}6$, $\omega = 105°$) by Labík and Nezbeda[27]. These data ($N = 216$, $N_c = (2-3) \times \times 10^6$, $N_c/N_a = 864$) are given in Table XIII. Their accuracy is about 1·5 per cent at small separations.

Tetrahedral Penta-atomics

Although realistic models of molecules with the tetrahedral symmetry have been the subject of several simulations, their simplest prototype, the FHS model, has been considered only in a study by Nezbeda and Voertler[38] ($L = 0{\cdot}52059$, $\sigma_B = = 1{\cdot}0294$; the inner sphere plays the role of an auxiliary site which contributes only

TABLE X
The fluid of hard heteronuclear diatomics (L=0.625, σ'_B=0.5): site-centred spherical harmonic expansion coefficients

$r_{\alpha\beta}/\sigma_{\alpha\beta}$	G^{AA}_{000}	G^{AB}_{000}	G^{BB}_{000}	G^{AA}_{100}	G^{AB}_{100}	G^{BA}_{100}	G^{BB}_{100}
			η = 0.25				
1.01	1.552	0.875	0.542	-0.411	-0.196	-0.749	-0.428
1.07	1.474	0.887	0.595	-0.302	-0.192	-0.704	-0.450
1.13	1.418	0.898	0.619	-0.220	-0.154	-0.650	-0.449
1.19	1.349	0.921	0.623	-0.139	-0.122	-0.612	-0.426
1.25	1.305	0.934	0.647	-0.065	-0.106	-0.559	-0.426
1.31	1.269	0.944	0.666	-0.003	-0.070	-0.514	-0.402
1.37	1.264	0.954	0.683	0.068	-0.053	-0.462	-0.399
1.39	1.239	0.964	0.689	0.068	-0.048	-0.442	-0.397
1.43	1.167	0.964	0.700	0.068	-0.023	-0.416	-0.391
1.47	1.115	0.983	0.711	0.057	-0.002	-0.387	-0.374
1.49	1.099	0.971	0.703	0.055	0.004	-0.363	-0.361
1.51	1.077	0.976	0.717	0.055	0.006	-0.342	-0.364
1.53	1.058	0.977	0.722	0.056	0.010	-0.326	-0.355
1.57	1.019	0.965	0.718	0.052	0.012	-0.291	-0.351
1.63	0.988	0.972	0.724	0.043	0.006	-0.245	-0.319
1.69	0.952	0.977	0.738	0.028	-0.002	-0.180	-0.316
1.75	0.923	0.977	0.751	0.021	-0.002	-0.133	-0.293
1.81	0.922	0.983	0.784	0.013	0.002	-0.081	-0.284
1.87	0.915	0.989	0.810	0.008	0.000	-0.040	-0.279
1.93	0.924	0.996	0.797	0.004	-0.006	0.014	-0.245
1.99	0.948	1.014	0.815	-0.004	-0.002	0.055	-0.240
2.05	0.972	1.022	0.829	-0.015	-0.012	0.102	-0.212
2.11	0.995	1.041	0.841	-0.015	-0.021	0.135	-0.203
2.15	1.000	1.062	0.860	-0.014	-0.006	0.174	-0.193
2.17	1.006	1.058	0.860	-0.016	-0.017	0.174	-0.187
2.19	1.009	1.049	0.871	-0.011	-0.019	0.166	-0.179
2.23	1.010	1.035	0.882	-0.011	-0.006	0.141	-0.174
2.29	1.023	1.024	0.903	-0.013	0.000	0.121	-0.162
2.35	1.022	1.019	0.910	-0.007	0.002	0.096	-0.138
2.41	1.024	1.017	0.930	0.000	0.004	0.067	-0.118
2.51	1.025	1.001	0.955	0.001	0.000	0.026	-0.094
2.61	1.013	1.000	0.979	0.002	0.008	0.000	-0.064
2.69	1.005	1.003	1.016	0.004	0.002	-0.018	-0.041
2.73	1.001	1.000	1.019	0.007	0.002	-0.018	-0.037
2.75	1.001	0.997	1.031	0.005	0.004	-0.022	-0.025
2.77	1.006	1.000	1.034	0.004	0.002	-0.020	-0.024
2.81	0.998	0.995	1.019	0.001	0.004	-0.030	-0.020
2.91	0.996	0.999	1.020	0.000	0.006	-0.034	-0.023
2.99	0.996	0.997	1.013	0.005	-0.002	-0.032	-0.011

TABLE X
(Continued)

$r_{\alpha\beta}/\sigma_{\alpha\beta}$	G^{AA}_{000}	G^{AB}_{000}	G^{BB}_{000}	G^{AA}_{100}	G^{AB}_{100}	G^{BA}_{100}	G^{BB}_{100}
			$\eta = 0.30$				
1.01	1.920	1.040	0.648	-0.459	-0.216	-0.874	-0.488
1.07	1.713	1.033	0.678	-0.322	-0.192	-0.793	-0.491
1.13	1.582	1.035	0.682	-0.223	-0.164	-0.716	-0.475
1.19	1.451	1.018	0.661	-0.118	-0.134	-0.637	-0.453
1.25	1.341	1.019	0.740	-0.043	-0.116	-0.573	-0.465
1.31	1.294	1.008	0.725	0.023	-0.069	-0.508	-0.420
1.37	1.232	1.006	0.758	0.064	-0.042	-0.443	-0.418
1.39	1.206	0.991	0.744	0.090	-0.034	-0.416	-0.400
1.43	1.137	1.004	0.751	0.083	-0.010	-0.380	-0.390
1.47	1.061	1.000	0.746	0.068	-0.002	-0.342	-0.377
1.49	1.047	1.000	0.748	0.070	0.016	-0.328	-0.370
1.51	1.011	1.002	0.773	0.065	0.026	-0.301	-0.376
1.53	0.988	0.994	0.769	0.056	0.026	-0.282	-0.360
1.57	0.964	0.990	0.775	0.063	0.022	-0.246	-0.346
1.63	0.915	0.973	0.779	0.043	0.018	-0.195	-0.326
1.69	0.895	0.964	0.784	0.029	0.010	-0.139	-0.310
1.75	0.878	0.974	0.797	0.024	0.012	-0.084	-0.290
1.81	0.883	0.966	0.816	0.010	0.012	-0.041	-0.273
1.87	0.893	0.973	0.815	0.004	-0.002	0.014	-0.246
1.93	0.932	0.992	0.818	-0.013	-0.006	0.058	-0.223
1.99	0.953	0.996	0.834	-0.014	-0.006	0.108	-0.211
2.05	0.984	1.012	0.836	-0.024	-0.010	0.148	-0.193
2.11	1.017	1.030	0.863	-0.019	-0.010	0.177	-0.180
2.15	1.026	1.048	0.867	-0.025	-0.013	0.214	-0.162
2.17	1.034	1.053	0.889	-0.014	-0.008	0.206	-0.164
2.19	1.037	1.047	0.888	-0.022	-0.017	0.201	-0.149
2.23	1.050	1.028	0.890	-0.014	-0.002	0.162	-0.137
2.29	1.039	1.019	0.912	-0.011	-0.002	0.120	-0.129
2.35	1.039	1.015	0.916	-0.002	-0.002	0.079	-0.109
2.41	1.037	1.013	0.943	0.000	0.000	0.045	-0.093
2.51	1.024	1.006	0.971	0.007	0.006	0.000	-0.065
2.61	1.005	1.005	0.994	0.007	-0.004	-0.028	-0.041
2.69	1.000	1.004	1.010	0.008	0.000	-0.036	-0.019
2.73	0.989	1.001	0.048	0.005	0.006	-0.050	-0.000
2.75	0.995	0.999	1.051	0.008	0.000	-0.042	-0.007
2.77	0.998	1.002	1.035	0.006	-0.004	-0.044	0.000
2.81	0.995	0.997	1.040	0.005	-0.002	-0.046	0.000
2.91	0.996	1.002	1.025	0.003	0.000	-0.044	-0.001
2.99	0.994	0.996	1.018	0.000	0.000	-0.040	0.000

TABLE X
(Continued)

$r_{\alpha\beta}/\sigma_{\alpha\beta}$	G^{AA}_{000}	G^{AB}_{000}	G^{BB}_{000}	G^{AA}_{100}	G^{AB}_{100}	G^{BA}_{100}	G^{BB}_{100}
			$\eta = 0.35$				
1.01	2.282	1.258	0.796	-0.545	-0.284	-1.039	-0.600
1.07	1.982	1.205	0.800	-0.355	-0.241	-0.904	-0.582
1.13	1.698	1.159	0.785	-0.205	-0.174	-0.786	-0.520
1.19	1.523	1.137	0.821	-0.107	-0.157	-0.694	-0.514
1.25	1.376	1.091	0.823	-0.011	-0.103	-0.596	-0.486
1.31	1.290	1.063	0.804	0.062	-0.068	-0.506	-0.457
1.37	1.222	1.040	0.792	0.121	-0.023	-0.414	-0.425
1.39	1.177	1.034	0.800	0.117	-0.027	-0.401	-0.415
1.43	1.095	1.013	0.817	0.101	0.010	-0.348	-0.413
1.47	1.013	1.022	0.828	0.087	0.012	-0.315	-0.397
1.49	0.976	1.005	0.816	0.077	0.040	-0.287	-0.375
1.51	0.948	1.009	0.804	0.074	0.036	-0.281	-0.358
1.53	0.934	0.995	0.802	0.065	0.036	-0.257	-0.352
1.57	0.893	0.978	0.804	0.060	0.023	-0.203	-0.338
1.63	0.842	0.948	0.796	0.040	0.028	-0.146	-0.314
1.69	0.834	0.955	0.824	0.030	0.017	-0.092	-0.300
1.75	0.836	0.941	0.825	0.015	0.024	-0.043	-0.267
1.81	0.846	0.942	0.817	0.003	0.009	0.021	-0.242
1.87	0.880	0.960	0.821	-0.017	-0.004	0.061	-0.228
1.93	0.929	0.965	0.838	-0.025	0.004	0.106	-0.205
1.99	0.983	0.988	0.837	-0.031	-0.012	0.146	-0.186
2.05	1.036	1.002	0.865	-0.037	-0.008	0.186	-0.166
2.11	1.072	1.035	0.867	-0.034	-0.023	0.213	-0.147
2.15	1.075	1.055	0.876	-0.023	-0.025	0.234	-0.139
2.17	1.077	1.062	0.878	-0.019	-0.019	0.244	-0.135
2.19	1.075	1.043	0.879	-0.020	-0.008	0.217	-0.121
2.23	1.080	1.029	0.902	-0.016	-0.014	0.187	-0.109
2.29	1.069	1.011	0.899	-0.005	-0.002	0.111	-0.093
2.35	1.051	1.008	0.910	-0.003	0.002	0.052	-0.077
2.41	1.039	1.018	0.948	0.008	-0.002	0.012	-0.065
2.51	1.017	1.006	0.972	0.011	0.004	-0.036	-0.040
2.61	0.984	1.007	1.008	0.012	0.004	-0.055	-0.009
2.69	0.977	1.011	1.038	0.014	0.004	-0.067	0.003
2.73	0.971	1.006	1.044	0.014	0.004	-0.066	0.006
2.75	0.975	1.007	1.044	0.009	0.006	-0.066	0.017
2.77	0.976	1.007	1.045	0.008	0.006	-0.070	0.021
2.81	0.971	1.004	1.041	0.005	0.002	-0.068	0.022
2.91	0.979	1.000	1.032	-0.005	0.004	-0.050	0.013
2.93	0.990	0.997	1.025	-0.006	0.002	-0.044	0.006

TABLE X
(Continued)

$r_{\alpha\beta}/\sigma_{\alpha\beta}$	G^{AA}_{000}	G^{AB}_{000}	G^{BB}_{000}	G^{AA}_{100}	G^{AB}_{100}	G^{BA}_{100}	G^{BB}_{100}
			$\eta = 0.40$				
1.01	2.957	1.543	0.986	-0.653	-0.299	-1.222	-0.721
1.07	2.229	1.419	0.936	-0.372	-0.233	-1.013	-0.651
1.13	1.811	1.333	0.992	-0.185	-0.189	-0.856	-0.641
1.19	1.530	1.234	0.936	-0.072	-0.138	-0.696	-0.561
1.25	1.329	1.166	0.889	0.025	-0.100	-0.585	-0.518
1.31	1.189	1.097	0.902	0.089	-0.039	-0.472	-0.474
1.37	1.128	1.058	0.875	0.157	-0.008	-0.383	-0.442
1.39	1.092	1.049	0.872	0.153	0.004	-0.359	-0.443
1.43	0.996	1.007	0.887	0.126	0.030	-0.308	-0.409
1.47	0.925	1.004	0.875	0.105	0.052	-0.253	-0.388
1.49	0.903	0.990	0.842	0.098	0.071	-0.242	-0.370
1.51	0.858	0.985	0.852	0.087	0.061	-0.217	-0.376
1.53	0.855	0.967	0.839	0.068	0.052	-0.188	-0.341
1.57	0.825	0.947	0.842	0.056	0.049	-0.140	-0.330
1.63	0.781	0.922	0.822	0.037	0.041	-0.092	-0.295
1.69	0.789	0.910	0.814	0.003	0.022	-0.040	-0.263
1.75	0.807	0.918	0.823	-0.008	0.024	0.020	-0.244
1.81	0.849	0.917	0.827	-0.013	0.009	0.059	-0.220
1.87	0.904	0.934	0.835	-0.033	0.009	0.101	-0.192
1.93	0.984	0.953	0.821	-0.040	0.006	0.147	-0.176
1.99	1.049	0.969	0.870	-0.042	-0.002	0.176	-0.155
2.05	1.109	0.997	0.862	-0.035	-0.012	0.191	-0.147
2.11	1.120	1.039	0.863	-0.027	-0.019	0.237	-0.121
2.15	1.119	1.051	0.867	-0.023	-0.021	0.254	-0.099
2.17	1.119	1.060	0.867	-0.017	-0.019	0.240	-0.100
2.19	1.102	1.047	0.867	-0.011	-0.019	0.209	-0.105
2.23	1.090	1.036	0.881	-0.002	-0.006	0.145	-0.075
2.29	1.068	1.020	0.900	-0.001	-0.006	0.067	-0.066
2.35	1.026	1.023	0.932	0.011	0.002	0.004	-0.046
2.41	1.014	1.035	0.948	0.021	-0.006	-0.043	-0.042
2.51	0.971	1.028	0.970	0.017	0.004	-0.080	-0.013
2.61	0.964	1.015	1.027	0.015	-0.002	-0.089	0.006
2.69	0.968	1.022	1.054	0.008	-0.004	-0.090	0.027
2.73	0.960	1.009	1.050	0.002	0.006	-0.081	0.033
2.75	0.958	1.004	1.081	0.003	-0.006	-0.072	0.044
2.77	0.958	1.002	1.065	-0.002	0.006	-0.074	0.033
2.81	0.976	1.000	1.045	-0.008	0.004	-0.070	0.027
2.91	0.992	0.996	1.037	-0.006	0.004	-0.044	0.005
2.99	1.012	0.995	1.015	-0.007	0.000	-0.024	-0.008

TABLE XI
Fluids of hard heteronuclear diatomics: average site-site correlation functions $G_{\alpha\beta}$

	L = 0.346, σ_B = 0.675					
	η = 0.3142			η = 0.4189		
$r_{\alpha\beta}$	G_{AA}	G_{AB}	G_{BB}	G_{AA}	G_{AB}	G_{BB}
0.675			0.254			0.438
0.700			0.281			0.485
0.750			0.384			0.591
0.800			0.485			0.689
0.850		0.694	0.586		1.104	0.774
0.875		0.761	0.637		1.124	0.813
0.900		0.820	0.686		1.151	0.852
0.950		0.929	0.781		1.229	0.934
0.975		0.978	0.830		1.253	0.979
1.000	1.985	1.022	0.881	2.987	1.263	1.022
1.025	1.886	1.064	0.931	2.767	1.273	1.064
1.050	1.822	1.099	0.978	2.529	1.272	1.106
1.100	1.758	1.150	1.071	2.181	1.261	1.193
1.150	1.706	1.189	1.170	1.932	1.257	1.270
1.200	1.602	1.229	1.227	1.685	1.263	1.278
1.250	1.454	1.267	1.215	1.421	1.272	1.215
1.275	1.380	1.285	1.202	1.304	1.281	1.179
1.300	1.312	1.299	1.190	1.202	1.285	1.144
1.350	1.197	1.287	1.165	1.037	1.239	1.082
1.375	1.147	1.254	1.148	0.969	1.179	1.052
1.400	1.101	1.207	1.130	0.914	1.108	1.027
1.450	1.023	1.107	1.094	0.836	0.979	0.989
1.500	0.964	1.033	1.059	0.779	0.893	0.960
1.550	0.917	0.979	1.022	0.740	0.838	0.932
1.600	0.879	0.932	0.988	0.730	0.815	0.910
1.700	0.854	0.889	0.941	0.763	0.826	0.903
1.800	0.863	0.898	0.927	0.847	0.901	0.932
1.825	0.872	0.905	0.929	0.876	0.924	0.943
1.850	0.882	0.913	0.932	0.907	0.948	0.956
1.875	0.894	0.923	0.936	0.940	0.972	0.968
1.900	0.908	0.934	0.940	0.974	0.993	0.980
2.000	0.982	0.979	0.967	1.109	1.053	1.022
2.100	1.043	1.012	1.001	1.174	1.080	1.047
2.200	1.068	1.034	1.022	1.140	1.078	1.050
2.300	1.057	1.040	1.026	1.059	1.048	1.033
2.400	1.037	1.031	1.027	0.982	1.009	1.009
2.500	1.008	1.015	1.013	0.938	0.970	0.987

TABLE XI
(Continued)

L=0.346, σ'_B=0.675, η=0.4712				L=0.75, σ'_B=0.5, η=0.4084			
$r_{\alpha\beta}$	G_{AA}	G_{AB}	G_{BB}	$r_{\alpha\beta}$	G_{AA}	G_{AB}	G_{BB}
0.675			0.575	0.500			1.458
0.700			0.618	0.550			1.319
0.750			0.725	0.600			1.176
0.800			0.800	0.650			1.071
0.850		1.380	0.874	0.700			0.971
0.875		1.393	0.898	0.750		2.017	0.903
0.900		1.389	0.927	0.800		1.738	0.857
0.950		1.377	0.988	0.850		1.495	0.816
0.975		1.369	1.024	0.900		1.315	0.796
1.000	3.783	1.364	1.068	0.950		1.168	0.794
1.025	3.387	1.351	1.100	1.000	3.505	1.058	0.794
1.050	2.954	1.328	1.141	1.050	2.697	0.972	0.807
1.100	2.362	1.280	1.218	1.100	2.116	0.913	0.830
1.150	1.984	1.256	1.277	1.150	1.699	0.883	0.853
1.200	1.677	1.256	1.290	1.200	1.403	0.869	0.878
1.250	1.325	1.247	1.172	1.225	1.290	0.867	0.891
1.275	1.192	1.241	1.136	1.250	1.198	0.866	0.904
1.300	1.073	1.245	1.099	1.275	1.122	0.865	0.918
1.350	0.904	1.216	1.031	1.300	1.059	0.864	0.934
1.375	0.842	1.113	0.995	1.350	0.969	0.867	0.970
1.400	0.781	1.007	0.968	1.400	0.919	0.880	1.004
1.450	0.706	0.880	0.935	1.450	0.908	0.899	1.045
1.500	0.666	0.809	0.908	1.475	0.910	0.912	1.066
1.550	0.650	0.766	0.905	1.500	0.908	0.926	1.079
1.600	0.657	0.765	0.887	1.525	0.897	0.943	1.080
1.700	0.738	0.829	0.907	1.550	0.880	0.961	1.073
1.800	0.900	0.942	0.954	1.600	0.843	0.993	1.049
1.825	0.942	0.975	0.964	1.650	0.831	1.029	1.028
1.850	0.998	1.005	0.983	1.700	0.834	1.077	1.009
1.875	1.030	1.032	0.998	1.725	0.839	1.098	1.000
1.900	1.067	1.057	1.010	1.750	0.848	1.109	0.992
1.950	1.140	1.088	1.039	1.775	0.861	1.108	0.985
2.000	1.212	1.108	1.055	1.800	0.878	1.030	0.910
2.100	1.236	1.105	1.068	1.900	0.959	1.046	0.972
2.200	1.133	1.073	1.051	2.000	1.075	1.009	0.976
2.300	1.001	1.026	1.017	2.100	1.108	0.983	0.988
2.400	0.915	0.967	0.981	2.200	1.072	0.976	0.999
2.500	0.874	0.935	0.961	2.300	1.027	0.976	1.003

TABLE XI
(Continued)

L = 0.75, η = 0.4084

σ_B=0.67				σ_B=0.84			
$r_{\alpha\beta}$	G_{AA}	G_{AB}	G_{BB}	$r_{\alpha\beta}$	G_{AA}	G_{AB}	G_{BB}
0.675			1.543	0.850			1.790
0.700			1.502	0.900			1.578
0.750			1.303	0.925		2.150	1.485
0.800			1.169	0.975		1.819	1.318
0.850		2.055	1.067	1.000	2.630	1.696	1.247
0.900		1.753	1.000	1.050	2.198	1.466	1.129
0.950		1.501	0.934	1.100	1.830	1.293	1.046
1.000	3.091	1.305	0.880	1.150	1.554	1.165	0.986
1.050	2.468	1.164	0.850	1.200	1.351	1.064	0.942
1.100	1.973	1.054	0.837	1.250	1.191	0.992	0.900
1.150	1.630	0.975	0.828	1.300	1.070	0.945	0.886
1.200	1.380	0.921	0.839	1.350	1.004	0.913	0.891
1.250	1.200	0.890	0.861	1.400	0.941	0.903	0.892
1.300	1.072	0.877	0.882	1.450	0.916	0.903	0.904
1.350	0.984	0.881	0.909	1.500	0.913	0.922	0.932
1.400	0.931	0.900	0.946	1.550	0.917	0.955	0.971
1.425	0.915	0.906	0.965	1.575	0.928	0.968	0.990
1.450	0.905	0.909	0.989	1.600	0.944	0.977	1.014
1.475	0.905	0.914	1.002	1.625	0.965	0.983	1.040
1.500	0.909	0.918	1.018	1.650	0.980	0.987	1.060
1.550	0.535	0.942	1.067	1.675	0.986	0.992	1.067
1.575	0.943	0.955	1.085	1.700	0.979	1.004	1.065
1.600	0.936	0.970	1.087	1.725	0.963	1.014	1.052
1.625	0.923	0.987	1.073	1.750	0.945	1.020	1.040
1.650	0.905	1.000	1.056	1.775	0.935	1.019	1.030
1.700	0.887	1.034	1.042	1.800	0.932	1.013	1.022
1.725	0.889	1.050	1.034	1.850	0.942	1.004	1.007
1.750	0.894	1.059	1.027	1.900	0.961	1.012	1.006
1.775	0.901	1.059	1.019	1.950	0.984	1.020	1.000
1.800	0.910	1.050	1.013	2.000	1.003	1.021	0.993
1.850	0.928	1.040	1.002	2.050	1.017	1.016	0.994
1.900	0.957	1.037	0.994	2.100	1.027	1.009	0.990
2.000	1.026	1.017	0.987	2.150	1.030	1.005	0.988
2.100	1.066	0.996	0.984	2.200	1.026	0.996	0.990
2.200	1.046	0.987	0.990	2.250	1.016	0.991	0.991
2.300	1.016	0.986	1.001	2.300	1.011	0.993	0.996
2.400	1.000	0.993	1.006	2.400	1.004	0.993	0.996
2.500	0.991	0.992	1.004	2.500	0.999	0.998	1.006

TABLE XII
The fluid of hard linear symmetric triatomics (L=0.8, σ_B=1): site-centred spherical harmonic expansion coefficients

$r_{\alpha\beta}$	G^{CC}_{000}	G^{CB}_{000}	G^{BB}_{000}	G^{CB}_{100}	G^{BB}_{100}
			η = 0.25		
1.01	0.342	0.687	1.091	-0.374	-0.517
1.05	0.421	0.721	1.083	-0.363	-0.485
1.09	0.467	0.751	1.081	-0.357	-0.446
1.13	0.539	0.784	1.069	-0.336	-0.414
1.17	0.558	0.808	1.056	-0.328	-0.367
1.21	0.605	0.826	1.051	-0.312	-0.341
1.25	0.626	0.841	1.047	-0.289	-0.308
1.29	0.686	0.858	1.040	-0.268	-0.272
1.33	0.703	0.888	1.029	-0.252	-0.236
1.37	0.768	0.906	1.034	-0.232	-0.212
1.41	0.789	0.911	1.035	-0.210	-0.177
1.45	0.799	0.956	1.033	-0.203	-0.147
1.47	0.850	0.953	1.049	-0.183	-0.134
1.48	0.856	0.956	1.051	-0.184	-0.117
1.51	0.866	0.969	1.052	-0.169	-0.109
1.53	0.907	0.974	1.033	-0.162	-0.096
1.55	0.912	0.974	1.031	-0.164	-0.095
1.59	0.932	0.986	1.001	-0.156	-0.091
1.63	0.975	1.000	0.975	-0.160	-0.081
1.67	1.008	1.020	0.959	-0.157	-0.077
1.71	1.035	1.026	0.934	-0.158	-0.071
1.75	1.071	1.051	0.923	-0.156	-0.067
1.77	1.115	1.058	0.908	-0.157	-0.065
1.79	1.138	1.067	0.910	-0.160	-0.066
1.81	1.130	1.063	0.903	-0.155	-0.060
1.83	1.119	1.051	0.897	-0.145	-0.064
1.85	1.120	1.044	0.901	-0.134	-0.056
1.89	1.115	1.031	0.900	-0.115	-0.058
1.95	1.114	1.008	0.897	-0.099	-0.053
2.01	1.080	0.996	0.904	-0.078	-0.050
2.11	1.057	0.984	0.921	-0.047	-0.050
2.21	1.049	0.978	0.943	-0.027	-0.043
2.31	1.044	0.981	0.970	-0.016	-0.034
2.41	1.022	0.985	0.994	-0.006	-0.021
2.51	1.020	0.996	1.021	0.004	-0.004
2.61	1.003	1.010	1.043	0.018	0.010

TABLE XII
(Continued)

$r_{\alpha\beta}$	G^{CC}_{000}	G^{CB}_{000}	G^{BB}_{000}	G^{CB}_{100}	G^{BB}_{100}
		η = 0.30			
1.01	0.447	0.847	1.318	-0.443	-0.608
1.05	0.527	0.867	1.292	-0.419	-0.558
1.09	0.596	0.888	1.245	-0.396	-0,496
1.13	0.647	0.906	1.219	-0.370	-0.449
1.17	0.674	0.917	1.181	-0.345	-0.394
1.21	0.712	0.927	1.151	-0.314	-0.349
1.25	0.735	0.938	1.127	-0.298	-0.310
1.29	0.765	0.940	1.104	-0.272	-0.267
1.33	0.791	0.946	1.083	-0.245	-0.227
1.37	0.822	0.959	1.073	-0.222	-0.192
1.41	0.846	0.965	1.068	-0.195	-0.156
1.45	0.861	0.981	1.063	-0.171	-0.115
1.47	0.885	0.993	1.065	-0.164	-0.098
1.49	0.892	1.001	1.071	-0.148	-0.081
1.51	0.913	1.001	1.074	-0.134	-0.063
1.53	0.924	1.004	1.052	-0.133	-0.059
1.55	0.937	1.008	1.029	-0.137	-0.056
1.59	0.989	1.007	0.991	-0.133	-0.054
1.63	1.013	1.021	0.961	-0.132	-0.048
1.67	1.053	1.027	0.933	-0.134	-0.042
1.71	1.083	1.035	0.911	-0.134	-0.042
1.75	1.116	1.051	0.895	-0.141	-0.040
1.77	1.130	1.060	0.887	-0.135	-0.038
1.79	1.167	1.069	0.885	-0.137	-0.038
1.81	1.156	1.063	0.878	-0.131	-0.038
1.83	1.138	1.056	0.873	-0.124	-0.040
1.85	1.147	1.044	0.876	-0.110	-0.039
1.89	1.117	1.016	0.867	-0.098	-0.040
1.95	1.094	0.991	0,879	-0.076	-0.040
2.01	1.074	0.977	0.893	-0.061	-0.045
2.11	1.055	0.969	0.924	-0.037	-0.046
2.21	1.030	0.972	0.957	-0.017	-0.042
2.31	1.023	0.981	0.988	-0.009	-0.032
2.41	1.027	0.984	1.015	-0.001	-0.018
2.51	1.014	0.997	1.036	0.014	-0.001
2.61	1.003	1.007	1.052	0.028	0.017

TABLE XII
(Continued)

$r_{\alpha\beta}$	G^{CC}_{000}	G^{CB}_{000}	G^{BB}_{000}	G^{CB}_{100}	G^{BB}_{100}
		$\eta = 0.35$			
1.01	0.611	1.077	1.605	-0.541	-0.727
1.05	0.711	1.089	1.511	-0.481	-0.633
1.09	0.793	1.060	1.442	-0.430	-0.554
1.13	0.802	1.060	1.357	-0.396	-0.476
1.17	0.849	1.028	1.290	-0.356	-0.405
1.21	0.812	1.020	1.233	-0.308	-0.351
1.25	0.873	1.009	1.191	-0.287	-0.300
1.29	0.858	1.004	1.144	-0.253	-0.251
1.33	0.865	0.992	1.112	-0.206	-0.203
1.37	0.893	0.984	1.083	-0.183	-0.160
1.41	0.870	0.986	1.072	-0.158	-0.117
1.45	0.905	0.999	1.062	-0.118	-0.076
1.47	0.889	1.002	1.070	-0.104	-0.051
1.49	0.916	1.005	1.072	-0.092	-0.033
1.51	0.932	1.012	1.069	-0.081	-0.013
1.53	0.940	1.009	1.045	-0.077	-0.013
1.55	0.963	1.011	1.012	-0.089	-0.008
1.59	0.977	1.011	0.973	-0.087	-0.007
1.63	1.026	1.013	0.930	-0.095	-0.014
1.67	1.051	1.015	0.897	-0.104	-0.016
1.71	1.097	1.028	0.876	-0.107	-0.018
1.75	1.118	1.039	0.858	-0.116	-0.022
1.77	1.147	1.048	0.846	-0.113	-0.021
1.79	1.175	1.063	0.847	-0.111	-0.022
1.81	1.161	1.057	0.843	-0.116	-0.025
1.83	1.156	1.035	0.835	-0.101	-0.026
1.85	1.128	1.022	0.840	-0.098	-0.026
1.89	1.096	1.001	0.841	-0.088	-0.029
1.95	1.073	0.958	0.860	-0.071	-0.043
2.01	1.032	0.957	0.887	-0.056	-0.046
2.11	1.019	0.965	0.938	-0.042	-0.055
2.21	1.019	0.976	0.979	-0.025	-0.051
2.31	1.022	0.979	1.011	-0.018	-0.037
2.41	1.015	0.993	1.035	-0.006	-0.017
2.51	1.017	1.006	1.053	0.012	0.004
2.61	1.006	1.016	1.065	0.024	0.027

TABLE XII
(Continued)

$r_{\alpha\beta}$	G_{000}^{CC}	G_{000}^{CB}	G_{000}^{BB}	G_{100}^{CB}	G_{100}^{BB}
			$\eta = 0.40$		
1.01	0.875	1.382	2.016	-0.668	-0.857
1.05	0.969	1.319	1.830	-0.568	-0.708
1.09	0.992	1.261	1.662	-0.494	-0.592
1.13	0.990	1.201	1.513	-0.430	-0.492
1.17	0.951	1.153	1.401	-0.374	-0.408
1.21	0.912	1.109	1.298	-0.326	-0.330
1.25	0.870	1.064	1.217	-0.281	-0.268
1.29	0.849	1.055	1.151	-0.251	-0.213
1.33	0.836	1.029	1.094	-0.209	-0.161
1.37	0.843	1.013	1.064	-0.173	-0.113
1.41	0.843	1.003	1.043	-0.135	-0.074
1.45	0.864	0.998	1.031	-0.097	-0.029
1.47	0.871	1.002	1.035	-0.076	-0.011
1.49	0.887	1.002	1.039	-0.054	-0.014
1.51	0.898	1.005	1.047	-0.042	0.037
1.53	0.920	1.005	1.016	-0.041	0.037
1.55	0.939	0.993	0.980	-0.049	0.031
1.59	0.989	0.982	0.923	-0.062	0.027
1.63	1.020	0.984	0.878	-0.072	0.019
1.67	1.060	0.985	0.842	-0.083	0.013
1.71	1.114	0.993	0.818	-0.102	0.005
1.75	1.171	1.009	0.808	-0.107	-0.001
1.77	1.210	1.019	0.805	-0.107	-0.001
1.79	1.217	1.033	0.806	-0.109	-0.004
1.81	1.219	1.028	0.802	-0.111	-0.010
1.83	1.187	1.004	0.799	-0.095	-0.012
1.85	1.160	0.982	0.811	-0.089	-0.015
1.89	1.106	0.957	0.822	-0.076	-0.025
1.95	1.064	0.949	0.857	-0.053	-0.043
2.01	1.049	0.959	0.908	-0.046	-0.060
2.11	1.019	0.975	0.978	-0.037	-0.074
2.21	1.008	0.984	1.019	-0.022	-0.063
2.31	1.003	0.990	1.035	-0.005	-0.045
2.41	1.009	0.999	1.058	0.006	-0.020
2.51	0.990	1.010	1.066	0.027	0.009
2.61	0.990	1.026	1.066	0.042	0.035

TABLE XIII

The fluid of hard non-linear symmetric triatomics (L=0.8, σ'_B=0.6, ω=105°): site-centered spherical harmonic expansion coefficients

r_{CC}	G^{CC}_{000}	r_{CB}	G^{CB}_{000}	G^{CB}_{100}	r_{BB}	G^{CB}_{000}	G^{CB}_{100}
			η = 0.25				
1.00	1.116	0.80	1.058	-0.681	0.60	0.984	-0.524
1.05	1.108	0.85	1.032	-0.609	0.65	0.959	-0.479
1.10	1.090	0.90	1.008	-0.549	0.70	0.936	-0.436
1.15	1.081	0.95	0.985	-0.500	0.75	0.915	-0.395
1.20	1.075	1.00	0.966	-0.458	0.80	0.900	-0.356
1.25	1.072	1.05	0.950	-0.417	0.85	0.881	-0.324
1.30	1.067	1.10	0.939	-0.379	0.90	0.863	-0.295
1.35	1.082	1.15	0.933	-0.345	0.95	0.848	-0.269
1.40	1.099	1.20	0.932	-0.313	1.00	0.836	-0.244
1.45	1.120	1.25	0.935	-0.284	1.05	0.828	-0.221
1.50	1.144	1.30	0.945	-0.257	1.10	0.823	-0.200
1.55	1.172	1.35	0.960	-0.230	1.15	0.824	-0.180
1.60	1.197	1.40	0.983	-0.206	1.20	0.829	-0.162
1.65	1.145	1.45	0.968	-0.174	1.25	0.838	-0.145
1.70	1.099	1.50	0.959	-0.140	1.30	0.845	-0.128
1.75	1.061	1.55	0.956	-0.108	1.35	0.865	-0.112
1.80	1.030	1.60	0.958	-0.077	1.40	0.886	
1.85	1.008	1.65	0.960	-0.043	1.45	0.904	
1.90	0.992	1.70	0.968	-0.010	1.50	0.932	
1.95	0.980	1.75	0.983	0.026	1.55	0.970	
2.00	0.972	1.80	1.004		1.60	1.012	
2.05	0.968	1.85	1.009		1.65	1.011	
2.10	0.967	1.90	1.012		1.70	1.008	
2.15	0.972	1.95	1.014		1.75	1.006	
2.20	0.975	2.00	1.018				
2.25	0.975	2.05	1.022				
2.30	0.977	2.10	1.022				
2.35	0.981	2.25	1.020				
2.40	0.986	2.20	1.018				
2.45	0.993	2.25	1.013				
2.50	0.999	2.30	1.009				
2.55	1.003	2.35	1.005				
2.60	1.006						
2.65	1.009						
2.70	1.011						
2.75	1.012						

TABLE XIII
(Continued)

r_{CC}	G^{CC}_{000}	r_{CB}	G^{CB}_{000}	G^{CB}_{100}	r_{BB}	G^{CB}_{000}	G^{CB}_{100}
			$\eta = 0.30$				
1.00	1.462	0.80	1.316	-0.796	0.60	1.213	-0.620
1.05	1.369	0.85	1.244	-0.692	0.65	1.137	-0.538
1.10	1.294	0.90	1.176	-0.601	0.70	1.074	-0.468
1.15	1.235	0.95	1.114	-0.524	0.75	1.024	-0.411
1.20	1.190	1.00	1.058	-0.458	0.80	0.983	-0.361
1.25	1.147	1.05	1.011	-0.402	0.85	0.941	-0.314
1.30	1.118	1.10	0.976	-0.353	0.90	0.903	-0.277
1.35	1.102	1.15	0.952	-0.311	0.95	0.872	-0.331
1.40	1.087	1.20	0.939	-0.274	1.00	0.847	-0.216
1.45	1.102	1.25	0.934	-0.244	1.05	0.829	-0.191
1.50	1.118	1.30	0.938	-0.216	1.10	0.818	-0.170
1.55	1.145	1.35	0.951	-0.191	1.15	0.816	-0.151
1.60	1.175	1.40	0.968	-0.166	1.20	0.823	-0.135
1.65	1.118	1.45	0.955	-0.137	1.25	0.834	-0.119
1.70	1.068	1.50	0.946	-0.102	1.30	0.848	-0.104
1.75	1.024	1.55	0.942	-0.074	1.35	0.866	-0.090
1.80	0.996	1.60	0.943	-0.046	1.40	0.889	
1.85	0.971	1.65	0.950	-0.015	1.45	0.913	
1.90	0.958	1.70	0.964	0.017	1.50	0.946	
1.95	0.958	1.75	0.986	0.054	1.55	0.986	
2.00	0.961	1.80	1.016		1.60	1.036	
2.05	0.963	1.85	1.017		1.65	1.030	
2.10	0.966	1.90	1.019		1.70	1.023	
2.15	0.970	1.95	1.021		1.75	1.020	
2.20	0.973	2.00	1.025				
2.25	0.975	2.05	1.027				
2.30	0.978	2.10	1.025				
2.35	0.983	2.25	1.019				
2.40	0.992	2.20	1.018				
2.45	0.998	2.25	1.014				
2.50	1.005	2.30	1.011				
2.55	1.011	2.35	1.007				
2.60	1.016						
2.65	1.018						
2.70	1.019						
2.75	1.018						

TABLE XIII
(Continued)

r_{CC}	G^{CC}_{000}	r_{CB}	G^{CB}_{000}	G^{CB}_{100}	r_{BB}	G^{CB}_{000}	G^{CB}_{100}
			$\eta = 0.35$				
1.00	1.882	0.80	1.677	-0.953	0.60	1.473	-0.707
1.05	1.689	0.85	1.504	-0.775	0.65	1.335	-0.591
1.10	1.522	0.90	1.355	-0.635	0.70	1.218	-0.495
1.15	1.380	0.95	1.230	-0.526	0.75	1.122	-0.413
1.20	1.264	1.00	1.124	-0.438	0.80	1.046	-0.342
1.25	1.174	1.05	1.044	-0.370	0.85	0.981	-0.292
1.30	1.111	1.10	0.981	-0.314	0.90	0.923	-0.249
1.35	1.074	1.15	0.937	-0.262	0.95	0.875	-0.214
1.40	1.056	1.20	0.910	-0.232	1.00	0.836	-0.185
1.45	1.056	1.25	0.901	-0.201	1.05	0.810	-0.160
1.50	1.074	1.30	0.905	-0.174	1.10	0.797	-0.141
1.55	1.110	1.35	0.928	-0.157	1.15	0.799	-0.125
1.60	1.151	1.40	0.953	-0.137	1.20	0.809	-0.112
1.65	1.085	1.45	0.938	-0.110	1.25	0.827	-0.100
1.70	1.030	1.50	0.931	-0.080	1.30	0.853	-0.089
1.75	0.987	1.55	0.930	-0.053	1.35	0.871	-0.076
1.80	0.957	1.60	0.935	-0.025	1.40	0.896	
1.85	0.948	1.65	0.949	0.005	1.45	0.927	
1.90	0.943	1.70	0.969	0.036	1.50	0.965	
1.95	0.943	1.75	0.999	0.072	1.55	1.011	
2.00	0.959	1.80	1.039		1.60	1.063	
2.05	0.969	1.85	1.034		1.65	1.051	
2.10	0.978	1.90	1.030		1.70	1.040	
2.15	0.985	1.95	1.032		1.75	1.034	
2.20	0.991	2.00	1.032				
2.25	0.995	2.05	1.030				
2.30	0.998	2.10	1.025				
2.35	0.999	2.25	1.018				
2.40	1.002	2.20	1.014				
2.45	1.008	2.25	1.012				
2.50	1.013	2.30	1.010				
2.55	1.017	2.35	1.005				
2.60	1.019						
2.65	1.020						
2.70	1.019						
2.75	1.017						

TABLE XIV

The fluid of hard tetrahedron penta-atomics (L=0.52059, σ_B=1.0294, V_m=2.1474): site-centred spherical harmonic expansion coefficients

	η = 0.2				η = 0.3			
$r_{\alpha\beta}/\sigma_{\alpha\beta}$	G_{CC}	G_{CB}	G_{BB}	G^{BB}_{100}	G_{CC}	G_{CB}	G_{BB}	G^{BB}_{100}
1.01			0.370	-0.346			0.565	-0.515
1.05			0.403	-0.364			0.586	-0.509
1.09		0.002	0.420	-0.367		0.004	0.600	-0.503
1.13		0.017	0.436	-0.367		0.029	0.604	-0.484
1.17		0.048	0.460	-0.367		0.076	0.619	-0.472
1.21		0.096	0.491	-0.380		0.159	0.636	-0.462
1.25		0.189	0.500	-0.370		0.297	0.648	-0.445
1.29		0.278	0.520	-0.367		0.428	0.662	-0.432
1.33		0.372	0.547	-0.365	0.001	0.556	0.681	-0.418
1.37	0.003	0.464	0.573	-0.366	0.008	0.682	0.695	-0.398
1.41	0.014	0.578	0.597	-0.358	0.036	0.801	0.719	-0.377
1.45	0.055	0.683	0.619	-0.346	0.111	0.929	0.742	-0.359
1.49	0.109	0.781	0.655	-0.345	0.217	1.043	0.762	-0.333
1.51	0.184	0.825	0.665	-0.336	0.304	1.100	0.780	-0.328
1.53	0.220	0.865	0.689	-0.333	0.385	1.155	0.789	-0.313
1.55	0.295	0.877	0.705	-0.325	0.487	1.125	0.801	-0.300
1.57	0.359	0.880	0.716	-0.313	0.611	1.122	0.822	-0.289
1.59	0.453	0.888	0.740	-0.311	0.745	1.117	0.843	-0.275
1.63	0.629	0.907	0.790	-0.292	0.950	1.098	0.888	-0.241
1.67	0.785	0.910	0.845	-0.260	1.188	1.085	0.956	-0.206
1.71	0.963	0.927	0.903	-0.232	1.362	1.070	1.029	-0.162
1.75	1.122	0.939	0.971	-0.202	1.534	1.064	1.096	-0.118
1.79	1.231	0.956	1.027	-0.163	1.677	1.056	1.163	-0.074
1.81	1.301	0.956	1.055	-0.141	1.704	1.052	1.202	-0.046
1.83	1.347	0.966	1.083	-0.128	1.713	1.056	1.220	-0.024
1.85	1.412	0.978	1.083	-0.117	1.751	1.063	1.206	-0.013
1.87	1.445	0.994	1.089	-0.107	1.744	1.067	1.195	-0.007
1.89	1.431	0.997	1.078	-0.099	1.740	1.079	1.180	-0.002
1.91	1.461	1.009	1.079	-0.090	1.764	1.085	1.169	0.011
1.93	1.484	1.027	1.072	-0.078	1.763	1.097	1.158	0.015
1.97	1.476	1.065	1.076	-0.062	1.674	1.137	1.137	0.031
2.03	1.451	1.127	1.066	-0.036	1.576	1.186	1.106	0.051
2.09	1.406	1.164	1.064	-0.013	1.395	1.216	1.082	0.061
2.15	1.306	1.191	1.062	0.013	1.300	1.240	1.059	0.087
2.21	1.260	1.206	1.059	0.035	1.228	1.217	1.046	0.103
2.27	1.204	1.187	1.060	0.059	1.116	1.186	1.033	0.119
2.39	1.113	1.125	1.056	0.110	0.986	1.081	1.026	0.139
2.51	1.047	1.064	1.063	0.148	0.895	0.987	1.027	0.184
2.71	0.963	0.995	1.020	0.116	0.850	0.911	0.983	0.094
2.91	0.938	0.963	0.985	0.072	0.870	0.919	0.964	0.028

TABLE XIV
(Continued)

$\eta = 0.4$

$r_{\alpha\beta}/\sigma_{\alpha\beta}$	G_{CC}	G_{CB}	G_{BB}	G_{100}^{BB}
1.01			0.906	-0.757
1.05			0.883	-0.704
1.09		0.010	0.858	-0.646
1.13		0.057	0.840	-0.602
1.17		0.145	0.818	-0.550
1.21		0.282	0.807	-0.512
1.25		0.494	0.791	-0.467
1.29		0.691	0.790	-0.435
1.33	0.001	0.851	0.783	-0.397
1.37	0.018	0.991	0.786	-0.362
1.41	0.088	1.119	0.790	-0.330
1.45	0.234	1.228	0.795	-0.293
1.49	0.470	1.323	0.817	-0.266
1.51	0.591	1.368	0.826	-0.251
1.53	0.738	1.392	0.838	-0.235
1.55	0.892	1.356	0.850	-0.221
1.57	1.061	1.321	0.864	-0.203
1.59	1.225	1.282	0.887	-0.186
1.63	1.492	1.216	0.956	-0.143
1.67	1.705	1.154	1.046	-0.091
1.71	1.856	1.114	1.136	-0.036
1.75	1.960	1.076	1.205	0.014
1.79	1.976	1.053	1.280	0.070
1.81	1.977	1.044	1.308	0.098
1.83	1.959	1.045	1.325	0.119
1.85	1.933	1.038	1.288	0.120
1.87	1.890	1.042	1.258	0.121
1.89	1.853	1.061	1.224	0.119
1.91	1.813	1.075	1.197	0.121
1.93	1.768	1.093	1.170	0.119
1.97	1.650	1.144	1.124	0.119
2.03	1.460	1.195	1.067	0.120
2.09	1.295	1.227	1.026	0.121
2.15	1.125	1.212	0.993	0.123
2.21	1.017	1.170	0.972	0.129
2.27	0.939	1.100	0.967	0.140
2.39	0.798	0.971	0.984	0.293
2.51	0.736	0.890	0.997	0.402
2.71	0.777	0.872	0.971	0.358
2.91	0.870	0.936	0.975	0.384

to the volume of the molecule, $V_m = 2{\cdot}1474 \pm 0{\cdot}0025$). They computed the average site–site correlation functions $G_{\alpha\beta}$ and one generalized coefficient, Γ^{BB}_{100}, required for evaluating the equation of state. These data ($N = 216$, $N_c = 2{\cdot}5 \cdot 10^6$, $N_c/N_a = 432$) are listed in Table XIV; their accuracy is about 2 per cent.

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