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VIRIAL COEFFICIENTS OF MORSE POTENTIAL

Using the numerical quadrature integration method and a modification of the Mayer sampling Monte Carlo technique proposed recently, the virial coefficients of the known three-parameter Morse potential have been calculated to the seventh order inclusive for potential parameter, αD, values of 3.0, 4.0, 6.0, 8.0, and 10.0. At low temperatures, a certain regularity in the behavior of the virial coefficients of all orders (beginning from the third one) is revealed for various αD-values. This regularity can be approximated by an equation similar to that previously obtained for the Lennard-Jones (12–6) and modified Lennard-Jones models.

Keywords: Morse potential, virial coefficient, irreducible cluster integral, Mayer sampling.

1. Introduction

One of the known theoretical approaches to describe dense states of matter is the virial equation of state [1–3]. Recently, another approach [4–8] has been proposed on the basis of the exact cluster expansion of the configuration integral, in which the equation of state also includes the so-called group irreducible integrals β_k or the virial coefficients associated with them [1],

$$B_{k+1} = -\frac{k}{k+1}\beta_k. \tag{1}$$

The corresponding equations of state can be exact only if they contain a complete set of coefficients ($k \to \infty$). Unfortunately, the problem of calculating the high-order irreducible integrals is connected with considerable technical difficulties even for the simplest model potentials of interaction between molecules. Modern computation methods allowed the irreducible integrals up to the sixth and even the seventh order – in Eq. (1), these are the virial coefficients up to the seventh and eighth, respectively, orders – to be determined with a certain accuracy in a limited temperature interval for the known Lennard-Jones (LJ) potential [9–11] and its modified (mLJ) version [12–14], the latter being more adapted to numerical experiments [15–17]. The results of those calculations even enabled a first attempt to approximate the infinite virial series for the LJ and mLJ potentials in the low-temperature interval [18]. However, the Lennard-Jones potential, as well as its modifications, reproduces the interaction between particles rather well only in inert gases.

Effective ionic interaction in various metals is simulated the most often [19, 20] by the three-parameter Morse potential [21]

$$U(r) = \varepsilon\left[e^{-2\alpha(r-D)} - 2e^{-\alpha(r-D)}\right], \tag{2}$$

where ε is the dissociation energy, and D the equilibrium distance between the particles. The presence of the third parameter α in Eq. (2) expands the application scope of this potential, but, at the same time, considerably complicates its theoretical and numerical researches. At present, information concerning the

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virial coefficients of the Morse potential is rather incomplete: irreducible integrals were calculated to the fourth order (and the virial coefficients to the fifth one) in a confined temperature interval and for three values of the parameter αD [22].

This work is aimed at calculating the virial coefficients of the Morse potential to the seventh order inclusive. A special attention is paid to the low-temperature interval in order to test the possibility to approximate the virial series of the Morse model, similarly to what was proposed recently for the LJ and mLJ models [18].

2. Calculation Technique

The irreducible integral of the k-th order, β_k, is defined as the sum of all possible products of Mayer functions $f(r) = \exp\left(-\frac{u(r)}{kT}\right) - 1$ for $k + 1$ molecules integrated over the configuration part of their phase space and divided by $k!V$, which is not expressed in terms of lower-order irreducible integrals [1]. Various combinations of such products are graphically represented by means of corresponding diagrams [23]. For each of the irreducible integrals of the first and second orders (in Eq. (1), these are the virial coefficients of the second and third orders), there exists only one such a diagram. However, the determination of the virial coefficients of the fourth, fifth, sixth, and seventh orders requires the calculation of 3, 10, 56, and 468 various integrals, respectively, in accordance with work [23].

A significant number of those integrals are simple enough to be calculated using the quadrature methods, as was proposed in work [12]. In such a way, all coefficients up to the fourth order can be calculated, and, partially, the others. More complicated integrals can be calculated, by using the modified method of Mayer sampling, which was described in detail in works [11, 13, 14]. The essence of this method is as follows.

A sought integral Γ (or a certain group of integrals) is determined, by using the already known (reference) integral Γ_0,

$$\Gamma = \Gamma_0 \frac{\langle \gamma/\pi \rangle_\pi}{\langle \gamma_0/\pi \rangle_\pi}. \tag{3}$$

Here, the notations γ and γ_0 mean integrands (a certain combinations of Mayer function products) for the sought and reference integrals, respectively; and the function π is the probability density for the given configuration (a point in the configuration space of molecules) to be accepted or rejected according to the Metropolis Monte-Carlo algorithm [24]. The sum of the absolute values of γ and γ_0 is used as the probability density π. The angular brackets in Eq. (3) mean the averaging over the whole ensemble of configurations.

This method differs, in principle, from the original Mayer sampling in that the simple integrals (previously determined by quadrature methods for the sought potential) rather than complicated ones (calculated for the hard-sphere potential) are used as references. This approach considerably reduces the computational costs and improves the calculation accuracy for the virial coefficients.

3. Calculation Results

The technique described above was used to calculate virial coefficients (1) in the dimensionless form $B^*_{k+1} = B_{k+1}/D^{3k}$ for the Morse potential (2), which was also reduced to the dimensionless form [25]

$$\frac{U(r)}{\varepsilon} = e^{-2\alpha^*\left(\frac{r}{D}-1\right)} - 2e^{-\alpha^*\left(\frac{r}{D}-1\right)}.$$

The calculations were carried out for various dimensionless temperatures $T^* = k_\mathrm{B}T/\varepsilon$ and the following values of the reduced parameter $\alpha^* = \alpha D$: 3.0, 4.0, 6.0, 8.0, and 10.0.

The coefficients B^*_2, B^*_3, and B^*_4 were integrated using the Gauss quadrature method. The same method was used to calculate 9 of 10 B^*_5-integrals, 41 of 56 B^*_6-integrals, and 206 of 468 B^*_7-integrals. The error was estimated by means of Aitken's process for 30, 60, and 120 integration nodes. All other (more complicated) integrals were calculated using the Mayer sampling. The resulting error consisted of the quadrature integration error and the standard error for the average of the Mayer sampling.

The results of calculations for the virial coefficients from the third to the seventh order are shown in Fig. 1 and in Appendix. In Fig. 1, the temperature, T^*, and virial coefficient, B^*_{k+1}, axes are presented on the logarithmic scale. As a result, one can easily detect a certain regularity in the behavior of those coefficients at various k and α^*. Despite a principle difference of the Morse potential from the LJ and mLJ

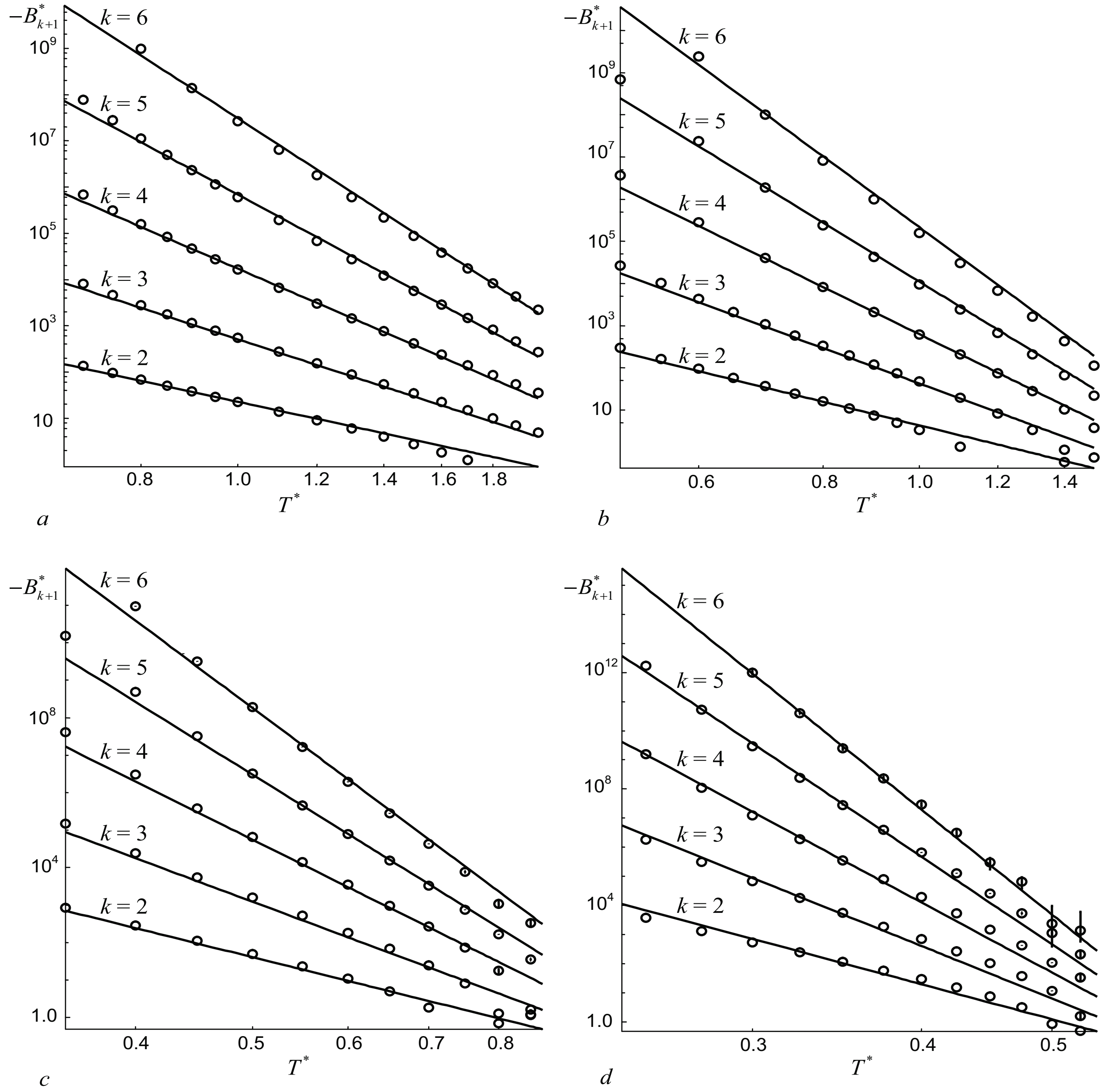

Fig. 1. Virial coefficients B^*_{k+1} of the Morse potential (circles; vertical segments show the 67% confidence interval) and their approximation (4) with function (5) for various values of parameter $\alpha^* = 3.0$ (*a*), 4.0 (*b*), 6.0 (*c*), and 10.0 (*d*)

ones, the behavior of virial coefficients at low temperatures turns out qualitatively similar for all those models.

In work [18], it was demonstrated that, in the case of LJ and mLJ models, the virial coefficient of any order $k \geq 2$ can be approximately determined by the equation

$$B^*_{k+1} = -\frac{a}{k\,(k-1)}\left[b\,(T^*)\right]^k. \qquad (4)$$

The analysis of the results of calculations performed in this work testifies that Eq. (4) remains

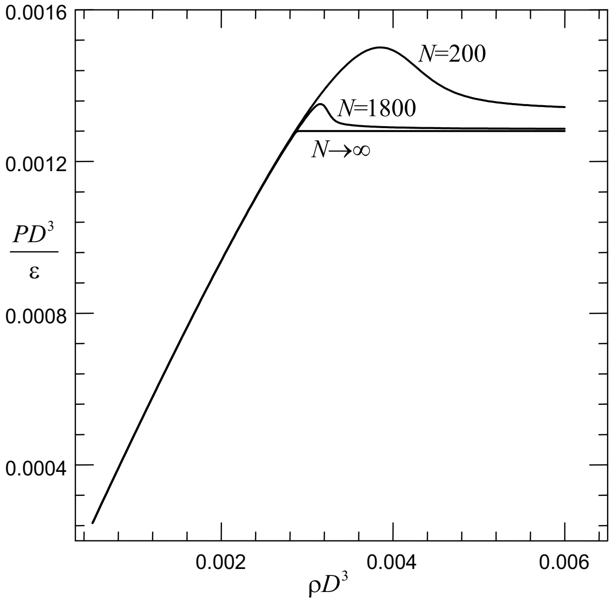

Fig. 2. Isotherms for a system with the Morse potential ($\alpha^* = 3.0$ and $T^* = 0.5$) and various numbers of particles, N, calculated on the basis of the exact cluster expansion of the configuration integral [4–6] and with the use of approximation (4)

valid for the coefficients of the Morse potential as well. Moreover, even the constant $a \approx 1/100$ in Eq. (4) remains the same as for the LJ and mLJ potentials at absolutely different values of the parameter α^* [18].

The search for the function $b\,(T^*)$ in Eq. (4) becomes somewhat complicated owing to the influence of the parameter α^*. The corresponding calculations show that, in a first approximation, this function may look like

$$b\,(T^*) = e^{5.25-0.825\alpha^*} T^{*-\frac{6+5\alpha^*}{9}}, \tag{5}$$

being qualitatively similar to $b\,(T^*)$ obtained in work [18] for the LJ and mLJ potentials. The behavior of approximation (4) with function (5) is compared with the actual $B^*_{k+1}\,(T^*)$-dependences in the same Fig. 1.

The extrapolation of Eq. (4) to the coefficients of higher orders allows the equations of state to be obtained on the basis of the exact cluster expansion of the configuration integral [4–6] for an arbitrary number of particles in the system (Fig. 2). As was shown in work [18], in the thermodynamic limit $N \to \infty$, the corresponding equation of state has the form

$$\frac{P}{k_{\mathrm{B}}T} = \begin{cases} \rho\,(1 - a + B_2\rho) + a\rho\,[1 - b\,(T)\,\rho] \times \\ \times\,[1 - \ln\{1 - b\,(T)\,\rho\}]\,; \quad \rho < \rho_0, \\ \rho_0\,(1 - a + B_2\rho_0)\,; \qquad \rho \geq \rho_0, \end{cases} \tag{6}$$

where $\rho_0 = [b\,(T)]^{-1}$. The isotherms of Eq. (6) have a discontinuity of the tangent at the condensation point ρ_0 (Fig. 2), which makes them qualitatively similar to isotherms of real substances.

4. Conclusions

To summarize, the virial coefficients of the Morse potential have been calculated for the first time up to the seventh order inclusive for various temperatures and potential parameter values $\alpha^* = 3.0$, 4.0, 6.0, 8.0, and 10.0. The data obtained allow the theoretical description of the dilute states of corresponding media to be made more accurate with the use of the virial equation of state or the exact cluster expansion of the configuration integral [4–8]. In addition, the analysis of the results obtained reveals a certain regularity [see Eq. (4)] in the behavior of virial coefficients at low temperatures. Earlier, this regularity was found only for the Lennard-Jones potential and its modified version [18]. On the one hand, such a regularity enables the virial coefficients to be interpolated on the basis of minimum information including a confined set of values for the parameter α^*. On the other hand, there is a possibility to extrapolate dependence (4) to higher-order coefficients (even to $k \to \infty$), as was proposed in work [18]. All that can facilitate and make much more exact the researches of various substances using the Morse potential with an arbitrary α^*.

Certainly, the general dependence (4) is, to a great extent, approximate, especially if rather a specific function (5) is taken into account, and requires further specifications as new data on the high-order virial coefficients, as well as coefficients for other potentials, will be accumulated. Most likely, such a specification should more concern the function $b\,(T^*)$ in Eq. (5) rather than the whole dependence (4), which means substantial quantitative, but not qualitative, changes in the corresponding equation of state (6).

APPENDIX

Dimensionless virial coefficients for the Morse potential, $B^*_{k+1} = B_{k+1}/D^{3k}$, at various values of reduced temperature $T^* = k_{\rm B}T/\varepsilon$ and parameter $\alpha^* = \alpha D$ (the numbers in parentheses indicate the 67%-confidence interval width corresponding to the least significant digit)

T^*	B^*_3	B^*_4	B^*_5	B^*_6	B^*_7
$\alpha^* = 3.0$					
0.20	$-2.7653799926\,(5) \times 10^{6}$	$-3.530\,(4) \times 10^{11}$	$-3.868\,(7) \times 10^{17}$	$-3.43\,(8) \times 10^{24}$	–
0.25	$-2.0332541089\,(7) \times 10^{5}$	$-2.4205\,(13) \times 10^{9}$	$-1.3530\,(19) \times 10^{14}$	$-3.28\,(3) \times 10^{19}$	–
0.30	$-3.57307380\,(3) \times 10^{4}$	$-9.781\,(3) \times 10^{7}$	$-8.438\,(9) \times 10^{11}$	$-2.123\,(10) \times 10^{16}$	–
0.35	$-1.011113912\,(6) \times 10^{4}$	$-1.0220\,(2) \times 10^{7}$	$-2.5317\,(19) \times 10^{10}$	$-1.414\,(2) \times 10^{14}$	–
0.40	$-3.81685889\,(8) \times 10^{3}$	$-1.8718\,(3) \times 10^{6}$	$-1.9149\,(11) \times 10^{9}$	$-3.710\,(3) \times 10^{12}$	$-1.3192\,(18) \times 10^{16}$
0.45	$-1.73887308\,(5) \times 10^{3}$	$-4.9076\,(5) \times 10^{5}$	$-2.5921\,(13) \times 10^{8}$	$-2.3079\,(14) \times 10^{11}$	–
0.50	$-902.19850\,(2)$	$-1.64200\,(14) \times 10^{5}$	$-5.176\,(2) \times 10^{7}$	$-2.5405\,(12) \times 10^{10}$	$-1.8618\,(15) \times 10^{13}$
0.55	$-514.297757\,(5)$	$-6.5386\,(5) \times 10^{4}$	$-1.3582\,(5) \times 10^{7}$	$-4.1486\,(18) \times 10^{9}$	–
0.60	$-314.6353616\,(3)$	$-2.96279\,(18) \times 10^{4}$	$-4.3523\,(16) \times 10^{6}$	$-9.017\,(4) \times 10^{8}$	$-2.5100\,(18) \times 10^{11}$
0.65	$-203.286948244\,(16)$	$-1.48217\,(8) \times 10^{4}$	$-1.6227\,(6) \times 10^{6}$	$-2.4273\,(10) \times 10^{8}$	–
0.70	$-137.142540\,(5)$	$-8.0146\,(4) \times 10^{3}$	$-6.807\,(3) \times 10^{5}$	$-7.701\,(4) \times 10^{7}$	$-1.1046\,(8) \times 10^{10}$
0.75	$-95.8007209\,(7)$	$-4.6132\,(2) \times 10^{3}$	$-3.1369\,(13) \times 10^{5}$	$-2.7839\,(14) \times 10^{7}$	–
0.80	$-68.860670\,(3)$	$-2.79460\,(17) \times 10^{3}$	$-1.5595\,(8) \times 10^{5}$	$-1.1177\,(5) \times 10^{7}$	$-9.793\,(8) \times 10^{8}$
0.85	$-50.684286\,(3)$	$-1.76637\,(14) \times 10^{3}$	$-8.261\,(4) \times 10^{4}$	$-4.891\,(2) \times 10^{6}$	–
0.90	$-38.055437\,(7)$	$-1.15696\,(13) \times 10^{3}$	$-4.614\,(2) \times 10^{4}$	$-2.2999\,(8) \times 10^{6}$	$-1.3682\,(16) \times 10^{8}$
0.95	$-29.058112\,(7)$	$-781.28\,(9)$	$-2.6947\,(12) \times 10^{4}$	$-1.1490\,(4) \times 10^{6}$	–
1.00	$-22.507884\,(8)$	$-541.58\,(6)$	$-1.6356\,(7) \times 10^{4}$	$-6.0453\,(18) \times 10^{5}$	$-2.618\,(3) \times 10^{7}$
1.10	$-13.983687\,(8)$	$-277.80\,(3)$	$-6.630\,(2) \times 10^{3}$	$-1.9028\,(4) \times 10^{5}$	$-6.312\,(7) \times 10^{6}$
1.20	$-9.004922\,(11)$	$-152.886\,(16)$	$-2.9782\,(10) \times 10^{3}$	$-6.8694\,(11) \times 10^{4}$	$-1.8120\,(18) \times 10^{6}$
1.30	$-5.948947\,(14)$	$-88.939\,(9)$	$-1.4506\,(5) \times 10^{3}$	$-2.7621\,(3) \times 10^{4}$	$-5.960\,(5) \times 10^{5}$
1.40	$-3.99718\,(3)$	$-54.100\,(6)$	$-754.0\,(2)$	$-1.21057\,(8) \times 10^{4}$	$-2.1854\,(18) \times 10^{5}$
1.50	$-2.70974\,(4)$	$-34.128\,(4)$	$-413.43\,(12)$	$-5.6951\,(9) \times 10^{3}$	$-8.757\,(6) \times 10^{4}$
1.60	$-1.83780\,(4)$	$-22.187\,(3)$	$-236.98\,(7)$	$-2.8403\,(8) \times 10^{3}$	$-3.777\,(2) \times 10^{4}$
1.70	$-1.23425\,(3)$	$-14.7892\,(18)$	$-141.01\,(4)$	$-1.4882\,(6) \times 10^{3}$	$-1.7322\,(9) \times 10^{4}$
1.80	$-0.80891\,(3)$	$-10.0668\,(13)$	$-86.62\,(2)$	$-813.1\,(4)$	$-8.373\,(3) \times 10^{3}$
1.90	$-0.50473\,(2)$	$-6.9735\,(9)$	$-54.691\,(14)$	$-460.61\,(14)$	$-4.2330\,(11) \times 10^{3}$
2.00	$-0.284624\,(19)$	$-4.9017\,(7)$	$-35.360\,(8)$	$-269.18\,(6)$	$-2.22539\,(15) \times 10^{3}$
$\alpha^* = 4.0$					
0.20	$-1.10370525\,(4) \times 10^{6}$	$-6.075\,(8) \times 10^{10}$	–	–	–
0.25	$-7.9303916\,(3) \times 10^{4}$	$-4.281\,(3) \times 10^{8}$	–	–	–
0.30	$-1.35595699\,(3) \times 10^{4}$	$-1.7473\,(6) \times 10^{7}$	$-5.325\,(13) \times 10^{10}$	$-3.289\,(16) \times 10^{14}$	$-3.59\,(3) \times 10^{18}$
0.35	$-3.71992629\,(3) \times 10^{3}$	$-1.8114\,(3) \times 10^{6}$	–	–	–
0.40	$-1.357093184\,(7) \times 10^{3}$	$-3.2485\,(3) \times 10^{5}$	$-1.3655\,(12) \times 10^{8}$	$-8.784\,(9) \times 10^{10}$	$-8.030\,(18) \times 10^{13}$
0.45	$-595.71793241\,(7)$	$-8.2628\,(5) \times 10^{4}$	–	–	–
0.50	$-296.884718\,(3)$	$-2.66429\,(11) \times 10^{4}$	$-3.6530\,(13) \times 10^{6}$	$-6.812\,(3) \times 10^{8}$	$-1.623\,(2) \times 10^{11}$
0.55	$-161.9971019\,(16)$	$-1.01713\,(3) \times 10^{4}$	–	–	–
0.60	$-94.486646\,(4)$	$-4.39918\,(10) \times 10^{3}$	$-2.8619\,(6) \times 10^{5}$	$-2.3857\,(7) \times 10^{7}$	$-2.406\,(3) \times 10^{9}$
0.65	$-57.927680\,(4)$	$-2.09213\,(4) \times 10^{3}$	–	–	–
0.70	$-36.870595\,(4)$	$-1.071184\,(17) \times 10^{3}$	$-4.0356\,(6) \times 10^{4}$	$-1.8770\,(5) \times 10^{6}$	$-1.0232\,(9) \times 10^{8}$
0.75	$-24.130265\,(4)$	$-581.426\,(8)$	–	–	–
0.80	$-16.108022\,(4)$	$-330.677\,(4)$	$-8.1465\,(11) \times 10^{3}$	$-2.4085\,(10) \times 10^{5}$	$-8.173\,(6) \times 10^{6}$
0.85	$-10.888504\,(6)$	$-195.269\,(2)$	–	–	–
0.90	$-7.399287\,(7)$	$-118.8451\,(14)$	$-2.0790\,(3) \times 10^{3}$	$-4.251\,(2) \times 10^{4}$	$-9.835\,(11) \times 10^{5}$
0.95	$-5.013694\,(9)$	$-74.0915\,(9)$	–	–	–

Continuation

T^*	B_3^*	B_4^*	B_5^*	B_6^*	B_7^*
1.00	−3.351857 (9)	−47.0599 (6)	−622.07 (9)	$-9.345\,(14) \times 10^{3}$	$-1.5625\,(19) \times 10^{5}$
1.10	−1.333852 (17)	−19.6821 (3)	−207.51 (4)	$-2.390\,(5) \times 10^{3}$	$-3.020\,(5) \times 10^{4}$
1.20	−0.27977 (2)	−8.33902 (18)	−74.34 (3)	−681 (2)	$-6.732\,(17) \times 10^{3}$
1.30	0.28552 (2)	−3.37079 (12)	−27.72 (2)	−208.8 (10)	$-1.639\,(9) \times 10^{3}$
1.40	0.59043 (2)	−1.12537 (8)	−10.40 (3)	−67.3 (5)	−426 (3)
1.50	0.751403 (15)	−0.10557 (6)	−3.776 (16)	−21.7 (3)	−113.6 (14)
1.60	0.830713 (10)	0.34241 (4)	−1.231 (10)	−7.27 (15)	−28.9 (7)
1.70	0.862934 (7)	0.51839 (3)	−0.290 (6)	−2.35 (10)	−6.5 (4)
1.80	0.867856 (6)	0.56497 (3)	0.015 (4)	−0.82 (6)	−1.30 (19)
1.90	0.857079 (5)	0.55169 (2)	0.077 (2)	−0.42 (4)	−0.12 (11)
2.00	0.837521 (4)	0.51294 (2)	0.0550 (15)	−0.33 (3)	−0.12 (12)
$\alpha^* = 6.0$					
0.20	$-3.03377\,(5) \times 10^{5}$	$-5.272\,(8) \times 10^{9}$	$-2.674\,(11) \times 10^{14}$	$-2.86\,(14) \times 10^{19}$	–
0.25	$-2.08200\,(5) \times 10^{4}$	$-3.784\,(5) \times 10^{7}$	$-1.482\,(4) \times 10^{11}$	$-9.83\,(9) \times 10^{14}$	–
0.30	$-3.35696\,(9) \times 10^{3}$	$-1.512\,(3) \times 10^{6}$	$-1.210\,(2) \times 10^{9}$	$-1.433\,(5) \times 10^{12}$	$-2.31\,(6) \times 10^{15}$
0.35	−857.68 (2)	$-1.484\,(2) \times 10^{5}$	$-4.068\,(8) \times 10^{7}$	$-1.516\,(8) \times 10^{10}$	$-7.23\,(9) \times 10^{12}$
0.40	−287.430 (8)	$-2.452\,(3) \times 10^{4}$	$-3.056\,(14) \times 10^{6}$	$-4.90\,(2) \times 10^{8}$	$-9.51\,(16) \times 10^{10}$
0.45	−113.960 (3)	$-5.613\,(7) \times 10^{3}$	$-3.794\,(15) \times 10^{5}$	$-3.204\,(17) \times 10^{7}$	$-3.15\,(5) \times 10^{9}$
0.50	−50.1404 (14)	$-1.5904\,(19) \times 10^{3}$	$-6.54\,(2) \times 10^{4}$	$-3.280\,(17) \times 10^{6}$	$-1.91\,(3) \times 10^{8}$
0.55	−23.3605 (8)	−518.9 (7)	$-1.404\,(5) \times 10^{4}$	$-4.55\,(2) \times 10^{5}$	$-1.66\,(3) \times 10^{7}$
0.60	−11.0245 (4)	−184.9 (3)	$-3.498\,(13) \times 10^{3}$	$-7.84\,(5) \times 10^{4}$	$-1.95\,(4) \times 10^{6}$
0.65	−4.9527 (3)	−68.67 (12)	−955 (4)	$-1.550\,(13) \times 10^{4}$	$-2.84\,(8) \times 10^{5}$
0.70	−1.82545 (19)	−25.08 (6)	−271.1 (13)	$-3.32\,(4) \times 10^{3}$	$-4.35\,(18) \times 10^{4}$
0.75	−0.17036 (13)	−8.02 (3)	−74.7 (5)	−757 (14)	$-7.7\,(5) \times 10^{3}$
0.80	0.71314 (10)	−1.301 (17)	−17.7 (19)	−165 (5)	$-1.08\,(13) \times 10^{3}$
0.85	1.17771 (8)	1.217 (10)	−1.62 (6)	−36 (2)	−330 (70)
0.90	1.40908 (7)	1.999 (6)	1.781 (18)	−9.9 (12)	−10 (30)
0.95	1.50875 (6)	2.075 (4)	1.682 (3)	−6.7 (6)	−31 (15)
1.00	1.53380 (6)	1.886 (3)	–	−4.6 (4)	0.9 (104)
$\alpha^* = 8.0$					
0.20	$-1.21513770\,(17) \times 10^{5}$	$-9.585\,(7) \times 10^{8}$	$-1.826\,(3) \times 10^{13}$	$-5.4\,(10) \times 10^{17}$	–
0.25	$-7.984743\,(6) \times 10^{3}$	$-6.891\,(14) \times 10^{6}$	$-1.0873\,(14) \times 10^{10}$	$-2.54\,(2) \times 10^{13}$	–
0.30	$-1.2115570\,(13) \times 10^{3}$	$-2.637\,(7) \times 10^{5}$	$-9.059\,(8) \times 10^{7}$	$-4.15\,(4) \times 10^{10}$	$-2.48\,(16) \times 10^{13}$
0.35	−285.38390 (13)	$-2.388\,(7) \times 10^{4}$	$-2.864\,(7) \times 10^{6}$	$-4.31\,(5) \times 10^{8}$	$-8.0\,(4) \times 10^{10}$
0.40	−85.67025 (3)	$-3.507\,(13) \times 10^{3}$	$-1.903\,(13) \times 10^{5}$	$-1.26\,(2) \times 10^{7}$	$-9.5\,(6) \times 10^{8}$
0.45	−29.002901 (13)	−681 (3)	$-1.962\,(16) \times 10^{4}$	$-6.71\,(16) \times 10^{5}$	$-2.7\,(2) \times 10^{7}$
0.50	−9.890321 (9)	−151.6 (11)	$-2.58\,(3) \times 10^{3}$	$-5.18\,(19) \times 10^{4}$	$-1.34\,(15) \times 10^{6}$
0.55	−2.717772 (7)	−33.3 (4)	−366 (5)	$-4.7\,(3) \times 10^{3}$	$-6.2\,(17) \times 10^{4}$
0.60	0.125016 (5)	−4.56 (19)	−42.7 (14)	−370 (60)	$-6\,(3) \times 10^{3}$
0.65	1.249978 (4)	2.02 (9)	1.39 (13)	−44 (15)	$-1.3\,(6) \times 10^{3}$
0.70	1.653371 (4)	2.91 (5)	3.32 (8)	−10 (4)	−100 (220)
0.75	1.745775 (4)	2.44 (3)	0.844 (12)	−11.1 (19)	−300 (1200)
0.80	1.705933 (4)	1.797 (16)	−0.745 (6)	−8.2 (10)	−30 (40)
0.85	1.614401 (4)	1.260 (10)	−1.361 (4)	−4.8 (5)	9 (14)
0.90	1.507964 (4)	0.870 (7)	−1.428 (3)	−2.3 (3)	14 (8)
0.95	1.403163 (4)	0.605 (4)	–	–	6 (4)
1.00	1.306951 (4)	0.433 (3)	–	–	2 (2)

End

T^*	B_3^*	B_4^*	B_5^*	B_6^*	B_7^*
			$\alpha^* = 10.0$		
0.20	$-5.9702448\,(11) \times 10^4$	$-2.5949\,(5) \times 10^8$	$-2.503\,(12) \times 10^{12}$	$-2.4\,(9) \times 10^{16}$	–
0.25	$-3.761185\,(5) \times 10^3$	$-1.84565\,(11) \times 10^6$	$-1.542\,(9) \times 10^9$	$-1.69\,(2) \times 10^{12}$	–
0.28	$-1.3235601\,(3) \times 10^3$	$-3.064256\,(13) \times 10^5$	$-1.115\,(4) \times 10^8$	$-5.31\,(7) \times 10^{10}$	–
0.30	$-535.41698\,(11)$	$-6.6966\,(3) \times 10^4$	$-1.2381\,(13) \times 10^7$	$-2.90\,(4) \times 10^9$	$-9.8\,(12) \times 10^{11}$
0.33	$-239.28227\,(7)$	$-1.7846\,(12) \times 10^4$	$-1.8688\,(18) \times 10^6$	$-2.44\,(5) \times 10^8$	$-4.1\,(4) \times 10^{10}$
0.35	$-114.69715\,(5)$	$-5.485\,(12) \times 10^3$	$-3.528\,(10) \times 10^5$	$-2.76\,(6) \times 10^7$	$-2.5\,(2) \times 10^9$
0.38	$-57.56067\,(4)$	$-1.872\,(6) \times 10^3$	$-7.84\,(4) \times 10^4$	$-3.94\,(11) \times 10^6$	$-2.3\,(3) \times 10^8$
0.40	$-29.56351\,(3)$	$-686\,(3)$	$-1.960\,(15) \times 10^4$	$-6.5\,(2) \times 10^5$	$-2.9\,(3) \times 10^7$
0.42	$-15.13540\,(3)$	$-262\,(2)$	$-5.30\,(6) \times 10^3$	$-1.27\,(5) \times 10^5$	$-3.1\,(6) \times 10^6$
0.45	$-7.41754\,(2)$	$-101.1\,(12)$	$-1.49\,(2) \times 10^3$	$-2.51\,(14) \times 10^4$	$-3.0\,(12) \times 10^5$
0.47	$-3.182838\,(17)$	$-37.3\,(7)$	$-414\,(11)$	$-5.2\,(4) \times 10^3$	$-6\,(3) \times 10^4$
0.50	$-0.827546\,(15)$	$-11.6\,(5)$	$-106\,(5)$	$-1.14\,(13) \times 10^3$	$2\,(12) \times 10^3$
0.53	$0.482324\,(13)$	$-1.5\,(3)$	$-33\,(8)$	$-210\,(50)$	$-1\,(5) \times 10^3$
0.55	$1.197215\,(11)$	$2.1\,(2)$	$1.8\,(13)$	$-40\,(20)$	$-1\,(2) \times 10^3$
0.57	$1.568194\,(9)$	$3.10\,(14)$	$4.3\,(6)$	$19\,(16)$	$3\,(3) \times 10^3$
0.60	$1.738859\,(8)$	$3.04\,(10)$	$2.7\,(3)$	$-7\,(6)$	$1.8\,(9) \times 10^3$
0.63	$1.793061\,(8)$	$2.62\,(7)$	$0.76\,(4)$	$-13\,(5)$	$-100\,(400)$
0.65	$1.780540\,(7)$	$2.12\,(5)$	$-0.568\,(10)$	$-7\,(4)$	$10\,(120)$
0.68	$1.731128\,(7)$	$1.66\,(4)$	$-1.321\,(5)$	$-9.6\,(18)$	$120\,(80)$
0.70	$1.662797\,(6)$	$1.27\,(3)$	$-1.640\,(3)$	$-5.7\,(14)$	$20\,(40)$

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ВІРІАЛЬНІ КОЕФІЦІЄНТИ ПОТЕНЦІАЛУ МОРЗЕ

Резюме

Із використанням квадратурних методів числового інтегрування у поєднанні з нещодавно запропонованим модифікованим методом вибірки Майера були розраховані віріальні коефіцієнти відомого трипараметричного потенціалу Морзе до сьомого порядку включно для різних значень параметра цього потенціалу αD: 3,0; 4,0; 6,0; 8,0; 10,0. В області низьких температур була виявлена певна закономірність у поведінці віріальних коефіцієнтів усіх порядків (починаючи з коефіцієнта третього порядку) при різних значеннях αD. Ця закономірність може бути апроксимована рівнянням, аналогічним тому, що було одержано раніше для потенціалу Ленард-Джонса (12–6) і модифікованого потенціалу Ленард-Джонса.