

Brigham Young University BYU ScholarsArchive

Faculty Publications

2006-04-14

Erratum: "Hard sphere radial distribution function again"

Andrij Trokhymchuk

Douglas Henderson

Ivo Nezbeda

Jan Jirsak

Follow this and additional works at: https://scholarsarchive.byu.edu/facpub



Part of the Biochemistry Commons, and the Chemistry Commons

Original Publication Citation

Trokhymchuk, Andrij, Ivo Nezbeda, Jan Jirsak, and Douglas Henderson. "Erratum: 'Hard sphere radial distribution function again" [J. Chem. Phys. [bold 123], 2451 (25)]." The Journal of Chemical Physics 124 (26).

BYU Scholars Archive Citation

Trokhymchuk, Andrij; Henderson, Douglas; Nezbeda, Ivo; and Jirsak, Jan, "Erratum: "Hard sphere radial distribution function again" (2006). Faculty Publications. 316. https://scholarsarchive.byu.edu/facpub/316

This Peer-Reviewed Article is brought to you for free and open access by BYU ScholarsArchive. It has been accepted for inclusion in Faculty Publications by an authorized administrator of BYU ScholarsArchive. For more information, please contact ellen_amatangelo@byu.edu.

Erratum: "Hard sphere radial distribution function again" [J. Chem. Phys. 123, 024501 (2005)]

Andrij Trokhymchuk^{a)}

Department of Chemistry and Biochemistry, Brigham Young University, Provo, Utah 84602

Ivo Nezbeda

E. Hála Laboratory of Thermodynamics, Institute of Chemical Process Fundamentals, Academy of Science, 165 02 Prague 6, Suchdol, Czech Republic and Department of Physics, J. E. Purkyně University, 400 96 Ústí nad Labem, Czech Republic

Jan Jirsák

E. Hála Laboratory of Thermodynamics, Institute of Chemical Process Fundamentals, Academy of Science, 165 02 Prague 6, Suchdol, Czech Republic

Douglas Henderson

Department of Chemistry and Biochemistry, Brigham Young University, Provo, Utah 84602

(Received 27 February 2006; accepted 28 February 2006; published online 14 April 2006)

[DOI: 10.1063/1.2188941]

Some misprints have been found for parameters $\mu \equiv \mu_o$ and $\gamma \equiv \gamma_o$ given by Eqs. (29) and (30) and the relevant equations in the Appendix. Both of these parameters can be evaluated directly using the original Wertheim solution¹ where they read

$$\mu\sigma \equiv \mu_o \sigma = \frac{2\eta}{1-\eta} \left(-1 - \frac{d}{2\eta} + \frac{\eta}{d} \right),\tag{29}$$

$$\gamma \equiv \gamma_o = \arctan \left\{ -\frac{1}{\beta_o} \frac{\left[\sigma(\alpha_o \left[\alpha_o^2 + \beta_o^2 \right] - \mu_o \left[\alpha_o^2 - \beta_o^2 \right] \right) \left(1 + \frac{1}{2} \eta \right) + \left(\alpha_o^2 + \beta_o^2 - \mu_o \alpha_o \right) (1 + 2 \eta) \right]}{\sigma(\alpha_o^2 + \beta_o^2 - 2\mu_o \alpha_o) \left(1 + \frac{1}{2} \eta \right) - \mu_o (1 + 2 \eta)} \right\}.$$

$$(30)$$

The calculations have been performed using correct equations and all results reported are not affected by these misprints.

The authors thank Monte Pettitt, Marcelo Marucho, Sorin Bastea, and Andreas Santos for their interest in the application of our equation that led to the discovery of the above misprints.

¹M. S. Wertheim, Phys. Rev. Lett. 10, 321 (1963).

a) Author to whom correspondence should be addressed. Permanent address: Institute for Condensed Matter Physics, National Academy of Sciences of Ukraine, Lviv 79011, Ukraine. Electronic mail: adt@icmp.lviv.ua