Zeitschrift für Physikalische Chemie Neue Folge, Bd. 75, S. 265–272 (1971)

Interconsistency of the *CHNC*, *PY* and Exact Theories Applied to Xenon

By

R. V. Gopala Rao and **K. Narasimhaswamy**

Department of Chemistry, S.V.U. College of Engineering, Tirupati (A.P.) India

With 6 figures

(Received March 15, 1971)

The interconsistency of *PY*, *CHNC* and exact theories in the calculation of the radial distribution function $g(r)$ for fluid xenon is tested by expanding it in power series up to $g_3(r)$ in the temperature range $T^* = 1 \cdot 2$ to 10. It is found that for the two particle densities for which calculations are made the peak height increased with decrease of temperature from $T^* = 10$ to $T^* = 2.5$. Discrepancies are observed at lower temperatures presumably due to the fact that the contribution from higher order terms is neglected. It is also found that the *PY* approximation yields a better fit with the exact theory than *CHNC* approximation.

The pressure calculations using upto the fifth virial coefficient are made and it is found that $\frac{PV}{RT}$ in the exact theory is nearer to *CHNC* theory in the low temperature region while the *PY* theory is better at higher temperatures.

Introduction

The study of the equilibrium properties of fluids has made rapid progress during the last few years especially in the calculation of the radial distribution function which is defined as the ratio of the local number density of molecules at a distance r from a fixed molecule to the average number density of molecules, $\varrho = N/V$. The radial distribution function is important as it is connected with the thermodynamic properties of the fluids. Of the several theories that have been put forward the *CHNC* and the *PY* theories received the greatest attention. In what follows, we discuss the interconsistency of the *CHNC*, *PY* and the exact graphic theories with applications to liquid xenon at various temperatures and particle densities.