

Isothermal Equations of State of Liquids and Intermolecular Potential Anisotropy

I. Adamenko, A. Grigoriev^{C, S} and Yu. Kuzovkov

Department of Physics, Kyiv Taras Shevchenko University, Kyiv, Ukraine

The isothermal K_T and adiabatic elasticity moduli K_S , thermal-expansion coefficient α_p , isochoric C_V and isobaric heat capacities C_p and their ratio γ of soft dumb-bell fluids were determined in Monte-Carlo simulations in a wide range of reduced densities and pressures. Atoms were assumed to interact through the soft sphere potential with exponent $m=12$. The distance between atoms L was varied from 0 to 0.6. Atom diameters were chosen so that molecular (dumb-bell) volume didn't change and was equal to 1. It was shown that at constant pressure the dependence of above mentioned thermophysical properties from L was much weaker than that of at constant density. Molecular nonsphericity was observed to not affect the pressure dependence of the elastic moduli. This may clarify the efficiency of fitting P - V - T data of a wide range of molecular liquids with isothermal equations of states such as Tait.