



## Computation of Some Thermodynamic Properties of Krypton-Xenon and Krypton-Neon Mixtures

Fluids

[Theory and Modeling](#)

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It is well known that a simple pair potential though giving the essential features of the thermodynamic properties of noble gases and their mixtures but it is not sufficient for a quantitative description and many-body effects most notably three-body interactions have to be taken into account. In fact, the structural and thermodynamic properties of fluids are influenced significantly by three-body interactions. Most works reported in the literature have been focused on three-body dispersion as calculated by Axilord and Teller [1]. Wang and Sadus [2] showed there is a simple empirical relationship between two-body and three-body interaction energies.

Wang and Sadus [2] showed that the addition of three-body interactions provides a near perfect agreement with experiment for the vapor branch of the existence curve while simultaneously improving the agreement with experiment on the liquid branch.

This work is the results of research conducted on the molecular dynamics simulation of the binary mixtures krypton-xenon and krypton-neon to obtain the pressure, internal energy, diffusion coefficient, and radial distribution function at different temperatures and densities. The Hartree-Fock dispersion (HFD)-like potential [3] and HFD-B potential [4], and Lennard-Jones (6,12) have been used as two-body potentials.

The simple expression of Wang and Sadus [2] has been used for incorporating the three-body interactions in our simulations with the HFD-like potential interactions. Our results show a very good agreement with the corresponding experimental data.

## References

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