Determination of Equation-of-State Parameters by Molecular Dynamics Simulations Combined with Quasi-chemical Nonrandom Lattice Fluid Model(QLF)

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Molecular dynamics simulations are used to determinate quasi-chemical nonrandom lattice fluid model(i.e., QLF)'s characteristic parameters P*, ρ*, T* of various substances. P*, ρ* are calculated by the cohesive energy density and density at 0 K, respectively. T* is determined by Boltzmann fitting. Lastly, estimated vapor pressure of various substances is compared with the experimental measurements.