Site-Site Potential Function and Second Virial Coefficients for Linear Molecules

Long Meng and Yuan-Yuan Duan
Key Laboratory for Thermal Science and Power Engineering of Ministry of Education, Tsinghua University, Beijing, China

The second virial coefficients for several linear molecules were calculated using the 2CLJ potential including the electrostatic and induction effects with modified mixing rules for unlike pairs. Least squares fits of experimental values for $B(T)$ were used to calculate the energy parameters $s$ and $e$ in the LJ core potential for $\text{N}_2$, $\text{O}_2$, $\text{Cl}_2$, $\text{F}_2$, $\text{CO}$, $\text{CO}_2$, $\text{NO}$, $\text{N}_2\text{O}$, $\text{C}_2\text{H}_6$, $\text{C}_2\text{F}_6$ and the strongly polar molecules $\text{CH}_3\text{Cl}$, $\text{CH}_3\text{F}$, $\text{CH}_3\text{CF}_3$, $\text{CH}_3\text{CHF}_2$, and $\text{CF}_3\text{CH}_2\text{F}$. The analysis takes into account rotation of the dipole out of the molecular axis. The calculated results for the second virial coefficient agree well with experimental data. In addition, the effect of the induction terms on the potential for calculating the second virial coefficient is shown to be important only for the molecules with strong dipole or quadrupole moments.

Keywords: Second virial coefficients; 2CLJ potential model; potential parameters; linear molecules