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

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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 N_2, O_2, Cl_2, F_2, CO, CO_2, NO, N_2O, C_2H_6, C_2F_6 and the strongly polar molecules CH_3Cl, CH_3F, CH_3CF_3, CH_3CHF_2, and CF_3CH_2F. 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