The form of the Lennard-Jones potential in lammps adopted as:

$$V_{ij}(r) = \begin{cases} 4\varepsilon_{ij}\left[(\frac{\sigma_{ij}}{r_{ij}})^{12} - (\frac{\sigma_{ij}}{r_{ij}})^{6}\right] & (r_{ij} \le r_{cutoff}) \\ 0 & (r_{ij} > r_{cutoff}) \end{cases}$$

where r_{ij} is the distance between two atoms; ε_{ij} and σ_{ij} are the energy and distance constants, respectively.

According to the Lorentz-Berthelot mixing rules, the energy and distance constants can be obtained in the following way:

$$\varepsilon_{ij} = \sqrt{\varepsilon_i \varepsilon_j}$$

$$\sigma_{ij} = \frac{\frac{1}{2}(\sigma_i + \sigma_j)}{\sqrt[6]{2}}$$

Of course, the last parameter that applies to lammps needs to be converted by unit.