

## van der Waals Parameters in Amber

There are two common formulations of the van der Waals equation:

$$E_{VDW} = 4\epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right] \quad \text{and} \quad E_{VDW} = 4\epsilon \left[ \frac{1}{4} \left( \frac{r_0}{r} \right)^{12} - \frac{1}{2} \left( \frac{r_0}{r} \right)^6 \right]$$

Both describe the non-bonded interaction between two particles at distance  $r$  as the sum of an attractive  $r^{-6}$  and a repulsive  $r^{-12}$  term. Two parameters are needed, the well depth  $\epsilon$  and a characteristic distance  $r_0$  or  $\sigma$  (the two formulations are identical for  $r_0 = \sqrt[6]{2}\sigma$ ). In the Amber forcefield, the later format is used, because of the easy physical interpretation of  $r_0$  as the energetically most favorable distance of two atoms.

In the parameter files, every atom type is given a radius and well depth parameter, e.g.

OH	1.7210	0.2104
CT	1.9080	0.1094

where the first number is the atomic radius in Angstrom and the second the well depth in kcal/mol. These values are then (at the time a *prmtop* file is written) combined to provide parameters for all pairs of atom types in the system:

$$r_{ij} = r_i + r_j \quad \text{and} \quad \epsilon_{ij} = \sqrt{\epsilon_i \epsilon_j}$$

These atom pair parameters are then used to calculate the ACOEFF and BCOEFF values in the *prmtop* file:

$$ACOEFF = \epsilon r_0^{12}; \quad BCOEFF = 2\epsilon r_0^6$$

E.g. for OH-CT non-bonded contacts, this gives:

$$ACOEFF = 7.91544157E+05$$

$$BCOEFF = 6.93079947E+02$$

The A and B coefficients are then used in sander's internal version of the VDW equation:

$$E_{VDW} = \frac{ACOEFF}{(r/\text{\AA})^{12}} - \frac{BCOEFF}{(r/\text{\AA})^6}$$