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 ε and a characteristic distance r_0 or σ (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:

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

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:

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

Thomas Steinbrecher, TSRI 2008 (steinbrt@scripps.edu)