Forcefields

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1 UFF

The theory presented here is adapted from Rappe et. al, JACS, 1992.

1.1 Bond distances

Equlibrium pairwise distances are given by

$$r_{ij} = r_i + r_j + r_{\mathrm{BO}} + r_{\mathrm{EN}} \tag{1}$$

where r_k is the covalant radius of atom k, r_{BO} a correction based on the bond order between the two atoms and r_{EN} a correction for the electronegativity.

$$r_{\mathrm{BO}} = -\lambda(r_i + r_j)\ln(n) \tag{2}$$

where $\lambda = 0.1332$ and n the bond order. For example, $n = 1.5$ for aromatic bonds.

$$r_{\mathrm{EN}} = r_i r_j \frac{(\sqrt{\chi_i} - \sqrt{\chi_j})^2}{\chi_i r_i \chi_j r_j} \tag{3}$$

where χ_k is the GMP electronegativity of atom k.

1.2 Force constants