$$V = \sum_{i} K_i (n_i - n_i)^2 + \sum_{i} K_i (\theta_i - \theta_i)^2 + \sum_{i} V_n [1 + \cos(n\phi_i - n_i)] + \sum_{i} \begin{bmatrix} A_{ij} & B_{ij} + q_i q_j \end{bmatrix}$$

 $U = \sum_{\text{bonds}} K_r (r - r_{\text{eq}})^2 + \sum_{\text{angles}} K_{\theta} (\theta - \theta_{\text{eq}})^2 + \sum_{\text{dihedrals}} \frac{V_n}{2} [1 + \cos(n\phi - \gamma)] + \sum_{i < j} \left[ \frac{A_{ij}}{r_{ij}^{12}} - \frac{B_{ij}}{r_{ij}^{6}} + \frac{q_i q_j}{\varepsilon r_{ij}} \right]$ 

non-bonded interactions

bend terms torsional terms

stretch terms