

Common Forcefield Terms and Their Derivatives

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1 Bond Stretching

These are interactions dealing with the radial distance between bonded atoms i and j . Define:

$$\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j \quad (1)$$

$$r_{ij} = |\mathbf{r}_{ij}| \quad (2)$$

1.1 Harmonic Bond Stretching

$$U_{ij} = k(r_{ij} - r_0)^2 \quad (3)$$

$$\frac{\partial U_{ij}}{\partial \mathbf{r}_i} = -\frac{\partial U_{ij}}{\partial \mathbf{r}_j} = 2k(r_{ij} - r_0) \frac{\mathbf{r}_{ij}}{r_{ij}} \quad (4)$$

2 Bond Bending

Interactions between 3 atoms (i , j , and k) in 2 consecutive bonds.

2.1 Harmonic Bond Bending

$$U_{ijk} = k(\theta_{ijk} - \theta_0)^2 \quad (5)$$

$$\frac{\partial U_{ijk}}{\partial \mathbf{r}_a} = 2k(\theta_{ijk} - \theta_0) \frac{\partial \theta_{ijk}}{\partial \mathbf{r}_a} \quad (6)$$

$$\frac{\partial \theta}{\partial \mathbf{r}_i} = \frac{1}{\sqrt{1 - \cos \theta}} \frac{1}{r_{ij}} \left[\frac{\mathbf{r}_{ij}}{r_{ij}} \cos \theta - \frac{\mathbf{r}_{kj}}{r_{kj}} \right] \quad (7)$$

$$\frac{\partial \theta}{\partial \mathbf{r}_k} = \frac{1}{\sqrt{1 - \cos \theta}} \frac{1}{r_{kj}} \left[\frac{\mathbf{r}_{kj}}{r_{kj}} \cos \theta - \frac{\mathbf{r}_{ij}}{r_{ij}} \right] \quad (8)$$

$$\frac{\partial \theta}{\partial \mathbf{r}_j} = -\frac{\partial \theta}{\partial \mathbf{r}_i} - \frac{\partial \theta}{\partial \mathbf{r}_k} \quad (9)$$

3 Dihedral Motion

3.1 Fourier Series

$$U_{ijkl} = \sum_n \frac{V_n}{2} [1 + \cos(n\omega_{ijkl} - \gamma)] \quad (10)$$

4 Non-bonded Interactions

4.1 Van der Waals

4.2 Electrostatic: Point/Point

5 Mixed Terms