

$$h_j(r_{ji}, r_{jk}, \theta_{ijk}) = \lambda \cdot \exp[r(r_{ji}-a)^{-1} + r(r_{jk}-a)^{-1}] \cdot (\cos \theta_{ijk} + \frac{1}{3})^2 \quad (6)$$

$$\cos \theta_{ijk} = \frac{\bar{r}_{ji}^2 + \bar{r}_{jk}^2 - \bar{r}_{ik}^2}{2 \times \bar{r}_{ji} \times \bar{r}_{jk}}$$

$$* \frac{\partial h_j}{\partial r_{ij}} = \lambda \cdot \exp[r(r_{ji}-a)^{-1} + r(r_{jk}-a)^{-1}] \cdot (-r)(r_{ji}-a)^{-2} \cdot (\cos \theta_{ijk} + \frac{1}{3})^2$$

$$+ \lambda \cdot \exp[r(r_{ji}-a)^{-1} + r(r_{jk}-a)^{-1}] \cdot 2(\cos \theta_{ijk} + \frac{1}{3}) \cdot \frac{(r_{ji}^2 - r_{jk}^2 + r_{ik}^2)}{2 \times r_{ij}^2 \times r_{jk}}$$

$$* \frac{\partial h_j}{\partial r_{ik}} = \lambda \cdot \exp[r(r_{ji}-a)^{-1} + r(r_{jk}-a)^{-1}] \cdot 2(\cos \theta_{ijk} + \frac{1}{3}) \cdot \frac{(-\bar{r}_{ik})}{\bar{r}_{ij} \times \bar{r}_{jk}}$$