

$$h_k(r_{ki}, r_{kj}, \theta_{ikj}) = \lambda \cdot \exp[r(r_{ik}-a)^{-1} + r(r_{kj}-a)^{-1}] \cdot (\cos\theta_{ikj} + \frac{1}{3})^2 \quad (7)$$

$$\cos\theta_{ikj} = \left( \frac{\bar{r}_{ik}^2 + \bar{r}_{jk}^2 - \bar{r}_{ij}^2}{2 \times \bar{r}_{ik} \times \bar{r}_{jk}} \right)$$

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

$$* \frac{\partial h_k}{\partial r_{ik}} = \lambda \cdot \exp[r(\bar{r}_{ik}-a)^{-1} + r(\bar{r}_{kj}-a)^{-1}] \cdot (-r)(\bar{r}_{ik}-a)^{-2} \cdot (\cos\theta_{ikj} + \frac{1}{3})^2$$

$$+ \lambda \cdot \exp[r(\bar{r}_{ik}-a)^{-1} + r(\bar{r}_{kj}-a)^{-1}] \cdot 2(\cos\theta_{ikj} + \frac{1}{3}) \cdot \frac{(\bar{r}_{ik}^2 - \bar{r}_{jk}^2 + \bar{r}_{ij}^2)}{2 \times \bar{r}_{ik} \times \bar{r}_{jk}}$$