④

* $U_3(i,j,k) = \varepsilon \cdot f_3\left(\frac{r_i}{\sigma}, \frac{r_j}{\sigma}, \frac{r_k}{\sigma}\right) = \varepsilon \cdot f_3(\bar{r_i}, \bar{r_j}, \bar{r_k})$

* $\dfrac{\partial U_3(i,j,k)}{\partial r_{ij}} = \dfrac{\partial U_3(i,j,k)}{\partial \bar{r}_{ij}} \cdot \dfrac{\partial \bar{r}_{ij}}{\partial r_{ij}} = \dfrac{\varepsilon}{\sigma} \cdot \dfrac{\partial f_3(\bar{r_i}, \bar{r_j}, \bar{r_k})}{\partial \bar{r}_{ij}}$

* $\dfrac{\partial U_3(i,j,k)}{\partial r_{ik}} = \dfrac{\varepsilon}{\sigma} \cdot \dfrac{\partial f_3(\bar{r_i}, \bar{r_j}, \bar{r_k})}{\partial \bar{r}_{ik}}$

* $f_3(\bar{r_i}, \bar{r_j}, \bar{r_k}) = h_i(r_{ij}, r_{ih}, \theta_{jik}) + h_j(r_{ji}, r_{jk}, \theta_{ijk}) + h_k(r_{ki}, r_{kj}, \theta_{ikj})$

$\dfrac{\partial f_3(\bar{r_i}, \bar{r_j}, \bar{r_k})}{\partial \bar{r}_{ij}} = \dfrac{\partial h_i}{\partial \bar{r}_{ij}} + \dfrac{\partial h_j}{\partial \bar{r}_{ij}} + \dfrac{\partial h_k}{\partial \bar{r}_{ij}}$

$\dfrac{\partial f_3(\bar{r_i}, \bar{r_j}, \bar{r_k})}{\partial \bar{r}_{ih}} = \dfrac{\partial h_i}{\partial \bar{r}_{ih}} + \dfrac{\partial h_j}{\partial \bar{r}_{ih}} + \dfrac{\partial h_k}{\partial \bar{r}_{ih}}$