

4th order Force Constants

$$\Phi_{ijkl}^{\alpha\beta\gamma\delta} = \frac{F_i^{\alpha} \left[\Delta r_j^{\beta}, \Delta r_k^{\gamma}, \Delta r_l^{\delta} \right] - F_i^{\alpha} \left[\Delta r_j^{\beta}, \Delta r_k^{\gamma} \right] - F_i^{\alpha} \left[\Delta r_k^{\gamma}, \Delta r_l^{\delta} \right] - F_i^{\alpha} \left[\Delta r_l^{\delta}, \Delta r_j^{\beta} \right] + F_i^{\alpha} \left[\Delta r_j^{\beta} \right] + F_i^{\alpha} \left[\Delta r_k^{\gamma} \right] + F_i^{\alpha} \left[\Delta r_l^{\delta} \right] - F_i^{\alpha,eq}}{\Delta r_j^{\beta} \Delta r_k^{\gamma} \Delta r_l^{\delta}}$$