The molecular potential energy surface V can be expressed in terms of normal coordinates q_r.

$$V = \frac{1}{2}\sum_r \omega_r q_r^2 + \frac{1}{6}\sum_{rst} \phi_{rst} q_r q_s q_t + \frac{1}{24}\sum_{rstu} \phi_{rstu} q_r q_s q_t q_u + ... \quad (1)$$

$$V = \frac{1}{2}\sum_r \omega_r q_r^2 + \frac{1}{6}\sum_{rst} k_{rst} q_r q_s q_t + \frac{1}{24}\sum_{rstu} k_{rstu} q_r q_s q_t q_u + ... \quad (2)$$

The number of force constants ϕ and k up to the quartic force field are given in columns 1 and 2. Only totally symmetrical force constants can be non-zero. The number of nonvanishing force constants k is given in the third column. (For optimized structures all first derivatives are zero. Since the normal coordinates are determinded by diagonalization of the force constant matrix the coupling constants ϕ_{ij} and k_{ij} $(i \neq j)$ are all zero. This simplifies the expression for V to the form given in equations (1) and (2).