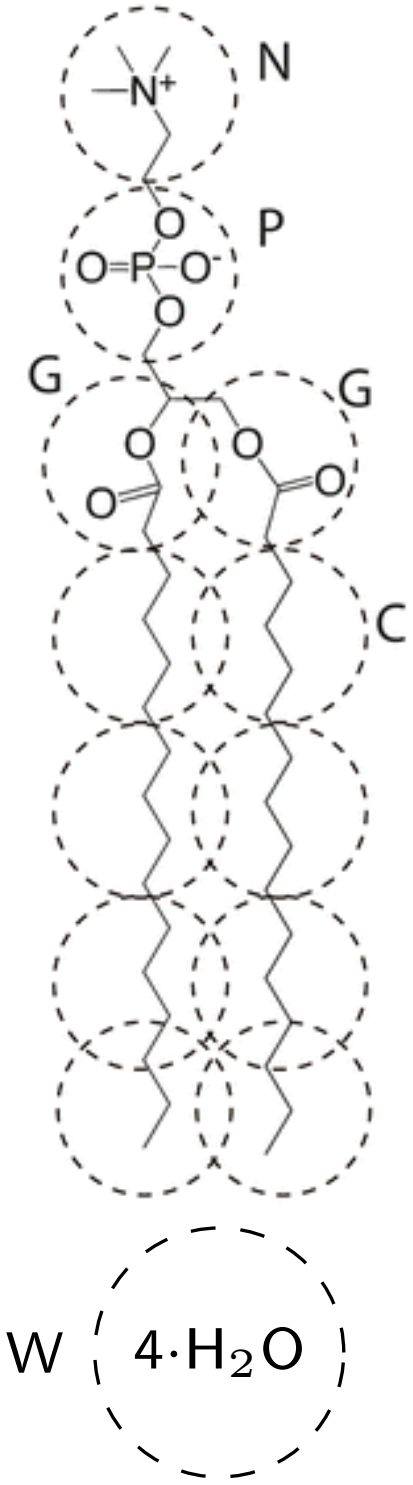
# CG-mapping




## Intramolecular hamiltonian

$$H_0 = \sum \frac{m_i \dot{\mathbf{r}}_i^2}{2} + \sum \frac{k_r (r_{ij} - r_0)^2}{2} + \sum \frac{k_\theta (\cos(\theta_{ijk}) - \cos(\theta_0))^2}{2}$$

## $W_1$-intercations

| G | P | C | W | |
|---|---|---|---|---|
| -1.50 | 6.30 | 9.00 | -8.10 | N |
| | 4.50 | 13.50 | -3.60 | P |
| $\tilde{\chi}_{k\ell}/\mathrm{kJ\,mol^{-1}}$ | | 6.30 | 4.50 | G |
| | | | 33.75 | C |

## New modeling of tension

$$W_1 = -\frac{1}{\rho_0} \int \mathrm{d}\mathbf{r}\; K_{\mathsf{ST}} \boldsymbol{\nabla}\phi_{\mathsf{W}}(\mathbf{r}) \cdot \boldsymbol{\nabla}\phi_{\mathsf{C}}(\mathbf{r})$$