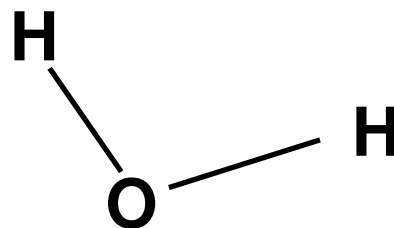
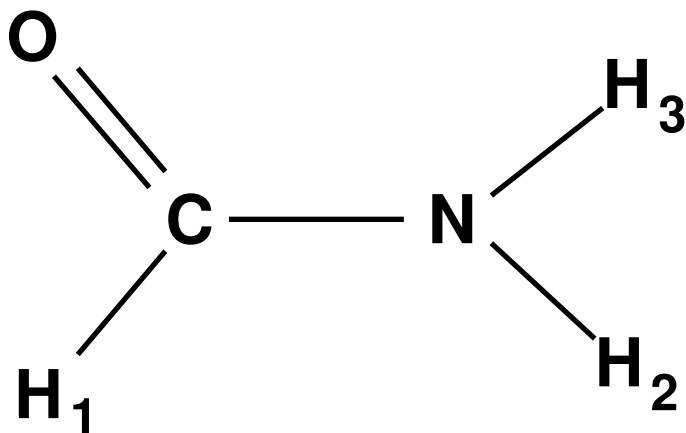


$$\begin{aligned}
 U = & \sum_{\text{bonds}} K_r (r - r_{eq})^2 + \sum_{\text{angles}} K_\theta (\theta - \theta_{eq})^2 + \sum_{\text{impropers}} K_w w^2 \\
 & + \sum_{\text{torsions}} K_\phi [1 + \cos(n\phi)] + \sum_{\text{nonbonded pairs}} \left\{ \left[\frac{B_{ij}}{r_{ij}^{12}} - \frac{A_{ij}}{r_{ij}^6} \right] + \frac{q_i q_j}{4\pi\epsilon_0 r} \right\}
 \end{aligned}$$



water



formamide