title

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Defining structure pool parameters

$$\mu \qquad \sigma_i$$

$$\rho$$

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$$\mu = 0, \text{ e.g. } \mathbf{R}_0$$

[picture of potential energy curve along a bond-distance, + bell curve vibrational distribution]
[and picture of $\mu \neq 0$ situation, shifted bell curve]

Defining structure pool parameters

$$\sigma = \begin{pmatrix} 0.4 \\ 0.2 \\ 0.2 \\ \vdots \\ 0.2 \end{pmatrix} \text{ Å}$$

- some displacements more important than others
- some could be irrelevant $\sigma_i = 0$ (i.e. don't displace at all)

Defining structure pool parameters

$$\rho \propto \text{accuracy} \;/\; \text{resolution}$$
$$\propto N$$
$$\propto 1/\sigma_i$$

NMM previous work

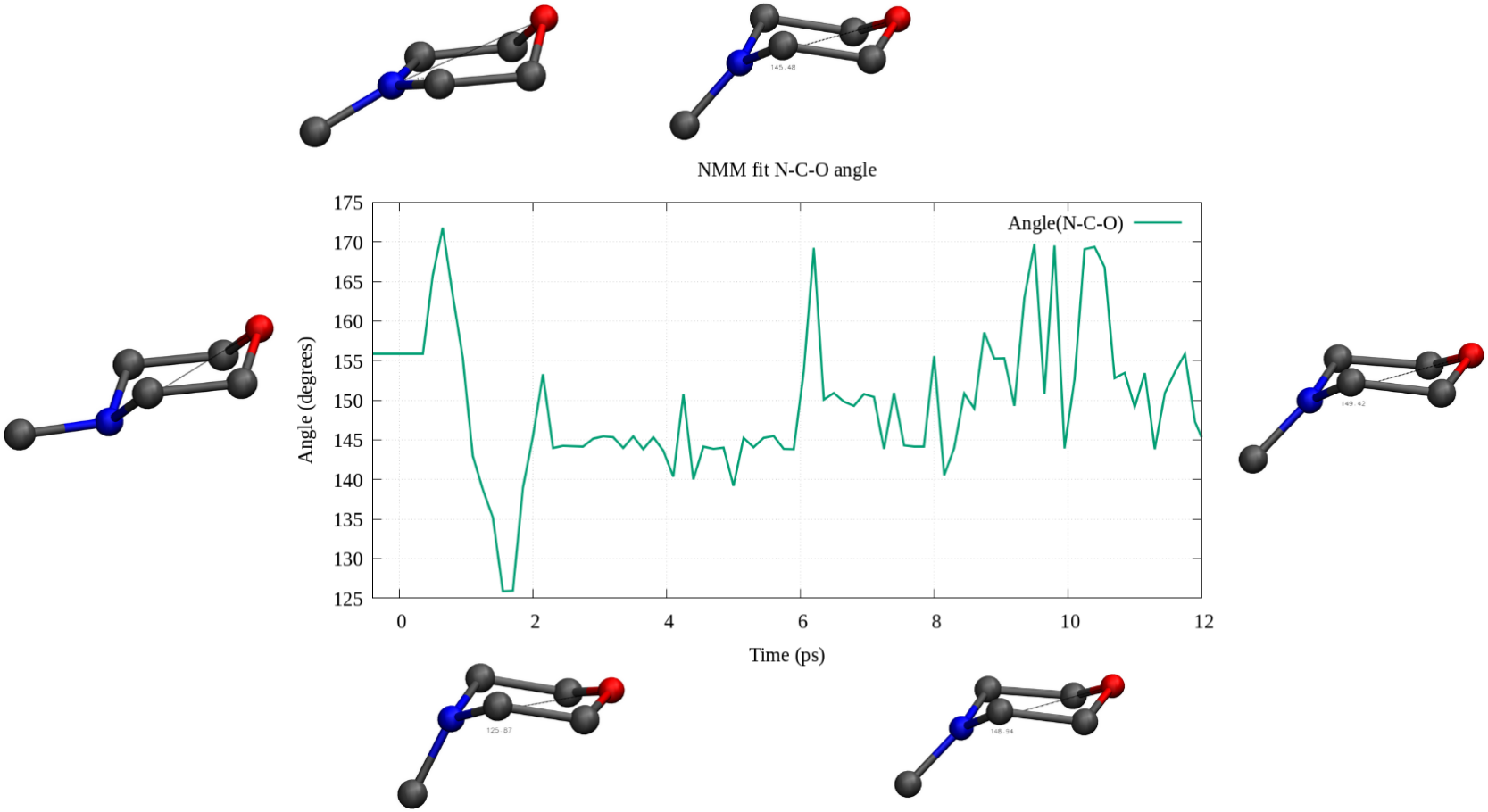

Figure: N-C-O angle of best fit to experiment trajectory.

Sampling method

The sampling equation for generating the displaced molecular coordinates is,

$$\mathbf{R} = \mathbf{R}_0 + \sum_{i}^{\text{modes}} a_i \mathbf{d}_i \tag{1}$$

with starting geometry $\mathbf{R}_0$, and displacement unit vectors $\mathbf{d}_i$ for each normal mode are obtained from a frequency calculation. The factors a_i are randomly generated within a bell curve centered at $\mu = 0$, and chosen standard deviation, σ.