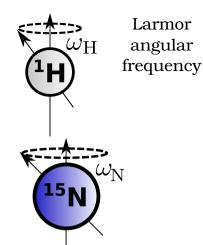
Redfield equations

Dipolar coupling constant

$$\begin{split} &\frac{1}{T_{1}} = \frac{d_{\mathrm{NH}}^{2}}{20} [J(\omega_{\mathrm{H}} - \omega_{\mathrm{N}}) + 3J(\omega_{\mathrm{N}}) + 6J(\omega_{\mathrm{H}} + \omega_{\mathrm{N}})] \\ &\frac{1}{T_{2}} = \frac{1}{2} \frac{d_{\mathrm{NH}}^{2}}{20} [4J(0) + J(\omega_{\mathrm{H}} - \omega_{\mathrm{N}}) + 3J(\omega_{\mathrm{N}}) + 3J(\omega_{\mathrm{H}}) + 6J(\omega_{\mathrm{H}} + \omega_{\mathrm{N}})] \\ &\mathrm{NOE} = 1 + \frac{d_{\mathrm{NH}}^{2}}{20} [J(\omega_{\mathrm{H}} + 6J(\omega_{\mathrm{H}} + \omega_{\mathrm{N}})] \frac{\gamma_{\mathrm{H}} T_{1}}{\gamma_{\mathrm{N}}} \end{split}$$



spectral density

$$J(\omega) = 2 \int_0^\infty C(t) \cos(\omega t) dt$$

Fourier transform second-order rotational correlation function of N-H bond vector

$$C(t) = \left\langle \frac{3}{2} \cos^2 \theta_{t'+t} - \frac{1}{2} \right\rangle_{t'}$$
 C(t

