Hydration water dynamics near d-NAGMA studied by DCS

Group B
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Outline

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5. Conclusion
Motivation

1. Protein hydration concerns:
   • the interaction between water and proteins
   • the structure and dynamics of water affected by proteins
2. Many techniques have been used to solve this problem:
   IR, NMR(MRD), X-ray, Neutron Scattering, Dielectric Resonance.
3. QENS could give more information regarding the dynamics of the hydration water near proteins.
4. Deuterated model peptides (NAGMA, 1.5M) are used to study water under various temperatures.

Methods

Disk Chopper Spectrometer (DCS)

Wavelength $\lambda = 7.5 \text{ Å}, 0.3 \text{ Å}^{-1} < Q < 1.5 \text{ Å}^{-1}$
Analysis of DCS data

Double differential cross section is proportional to the incoherent scattering:

\[
\frac{d^2 \sigma}{dE d\Omega} = \frac{\sigma_{in} k_s}{4\pi k_i} NS_{inc} (Q, \omega)
\]

\(S_{inc}\) is a convolution of vibrational, translational and rotational motions:

\[
S_{inc} (Q, \omega) = e^{-\langle u^2 \rangle Q^2 / 3} S_{inc}^{trans} (Q, \omega) \otimes S_{inc}^{rot} (Q, \omega)
\]

Fitting with 2 Lorentzian functions.

\[
\Gamma_{trans} (Q) = \frac{D_{trans} Q^2}{1 + D_{trans} Q^2 \tau_0}
\]

M Bee, Quasielastic Neutron Scattering, Adam Hilger, 1988
D Russo, R Murarka, J Copley, T Head-Gordon, JPCB 109, 12966 (2005).
Two Lorentzian fitting

273K, $|Q|^{-1} = 0.86951 \text{ Å}$

$|Q|^{(-1)} = 0.86951$

310K, $|Q|^{-1} = 0.94614 \text{ Å}$

$|Q|^{(Å^{-1})} = 0.94614$
KWW stretched exponential (SE)

\[
S_{inc} (Q, t) = e^{-\langle u^2 \rangle^{2/3}} \exp \left[-\left(\frac{1}{\tau_\alpha (Q, T)}\right)^{\beta(Q,T)}\right]
\]

273K, $|Q|^{-1}=0.86951$ Å, $\beta=0.7784$

310K, $|Q|^{-1}=0.94614$ Å, $\beta=0.8468$
Translation diffusion vs. Temperature

\[ \Gamma_{trans}(Q) = \frac{D_{trans}Q^2}{1 + D_{trans}Q^2\tau_0} \]

\[ \frac{1}{\tau} = \frac{\tau_\alpha}{\beta} \Gamma \text{ammaFunc}\left(\frac{1}{\beta}\right) \]

<table>
<thead>
<tr>
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<th>( E_a ) (kJ/mol)</th>
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<tbody>
<tr>
<td>( \text{WATER} )</td>
<td>NAGMA</td>
</tr>
<tr>
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<tr>
<td>( \text{SE} )</td>
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Conclusions

Study of the water dynamic around proteins:

• Two models:
  – Fitting with 2 Lorentzian: take into consideration translational and rotational motions;
  – Stretched exponential (KWW): just translational part rotation?
    solution: increase resolution through lower q or intensity decrease.

• Diffusion is slower than bulk water in the temperature range of our study.
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