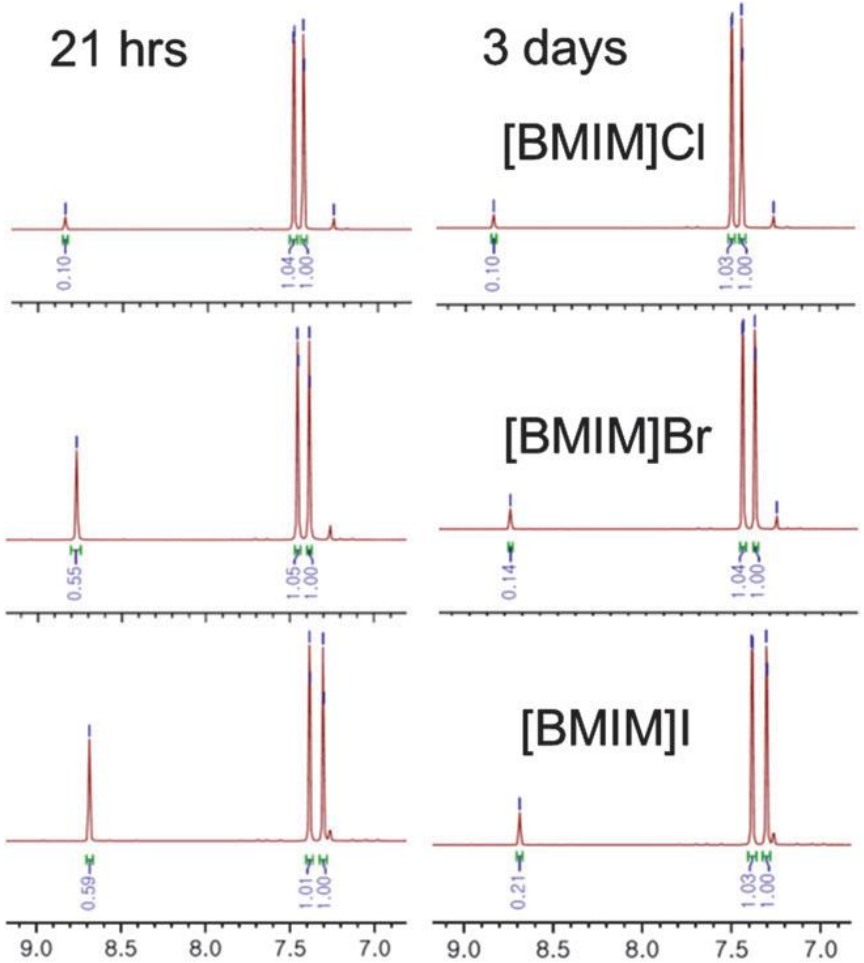
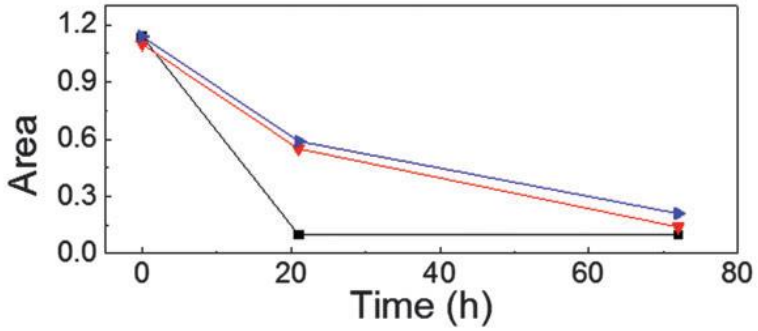
Isotopic substitution of imidazolium-based ionic liquids





$$H_2O + D_2O \leftrightarrows 2HOD$$

Instantaneous ~ ps

So slow
Why?

SCIENTIFIC REPORTS

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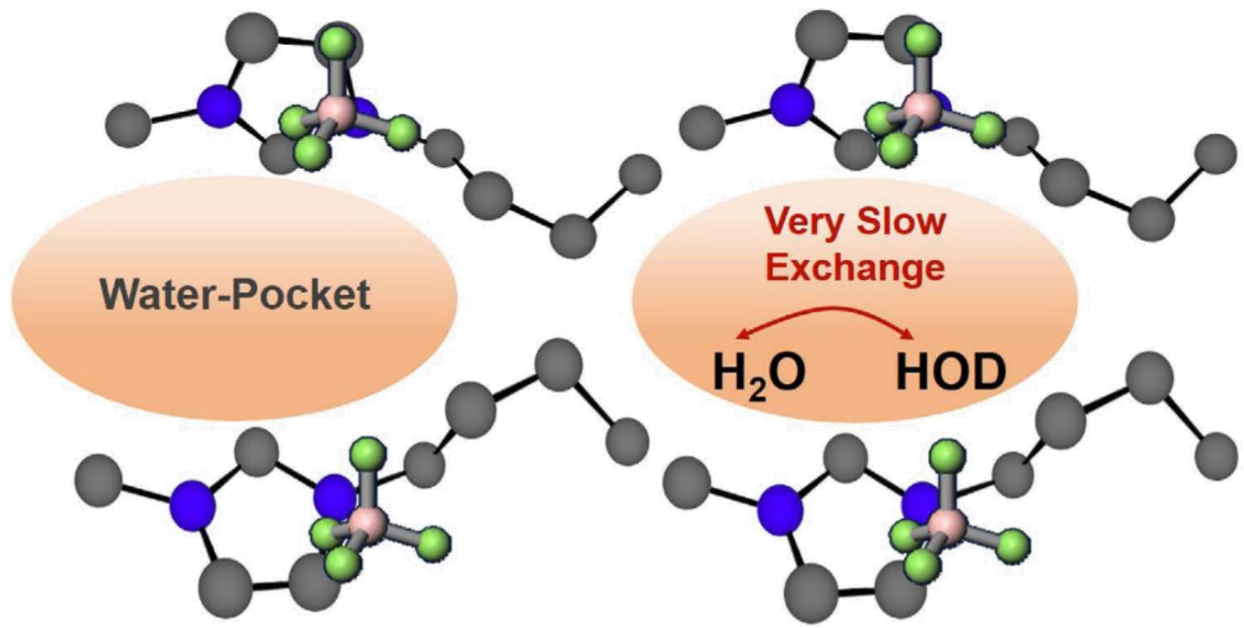
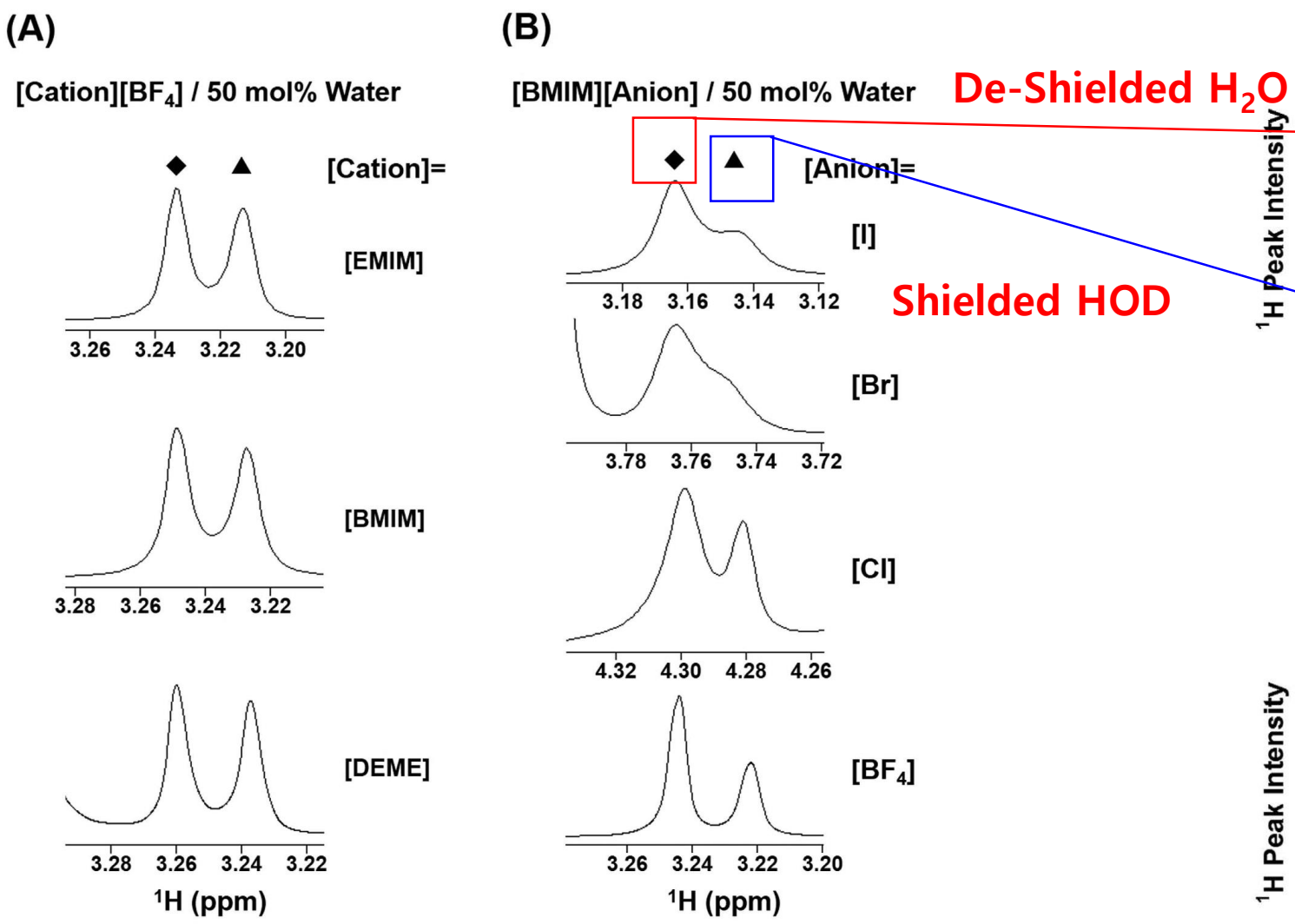
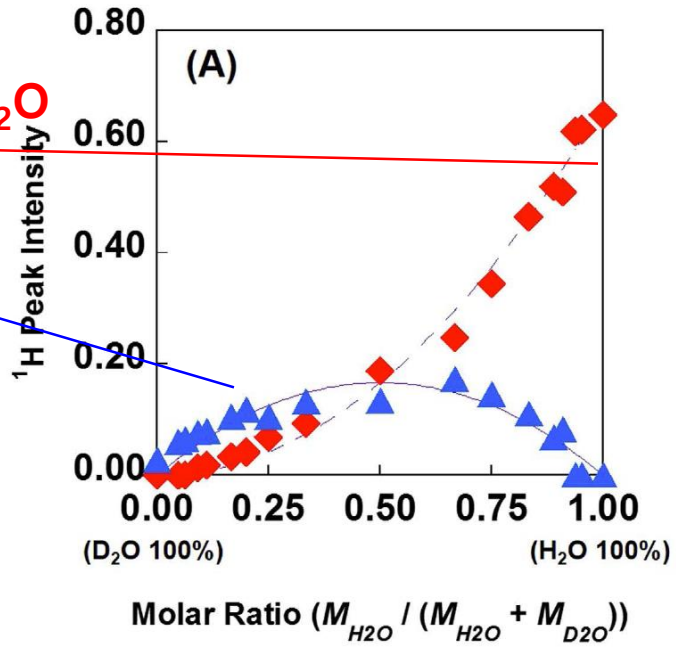
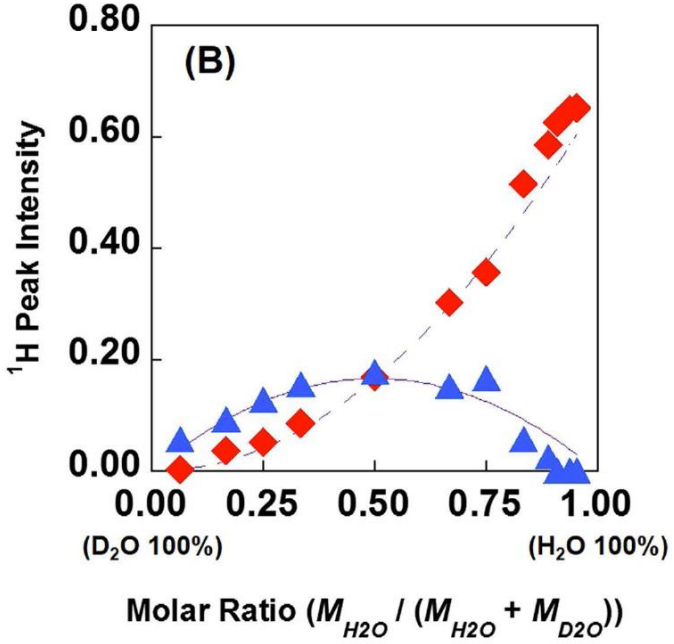
Properties of Water Confined in Ionic Liquids

Koji Saihara[1], Yukihiro Yoshimura[2], Soichi Ohta[1] & Akio Shimizu[1]









Separated ^{1}H peak of Shielded water / Deshields water

→ Abnormally slow proton exchange

→ Water-Pocket

	Self-diffusion coefficient (m^2/s)
H_2O for 1:1 H_2O:D_2O	**2.25×10^{-9}**
HOD for 1:1 H_2O:D_2O	**2.11×10^{-9}**
H_2O for 1:0.5:0.5 [BMIM][BF_4]:H_2O:D_2O	**4.39×10^{-10}**
HOD for 1:0.5:0.5 [BMIM][BF_4]:H_2O:D_2O	**4.33×10^{-10}**
$[BMIM]^+$ for 1:0.5:0.5 [BMIM][BF_4]:H_2O:D_2O	6.63×10^{-11}
$[BF_4]^-$ for 1:0.5:0.5 [BMIM][BF_4]:H_2O:D_2O	7.08×10^{-11}

THE JOURNAL OF PHYSICAL CHEMISTRY Letters

Letter

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Nanoconfinement's Dramatic Impact on Proton Exchange between Glucose and Water

Benjamin P. Wiebenga-Sanford, Joseph DiVerdi, Christopher D. Rithner, and Nancy E. Levinger*

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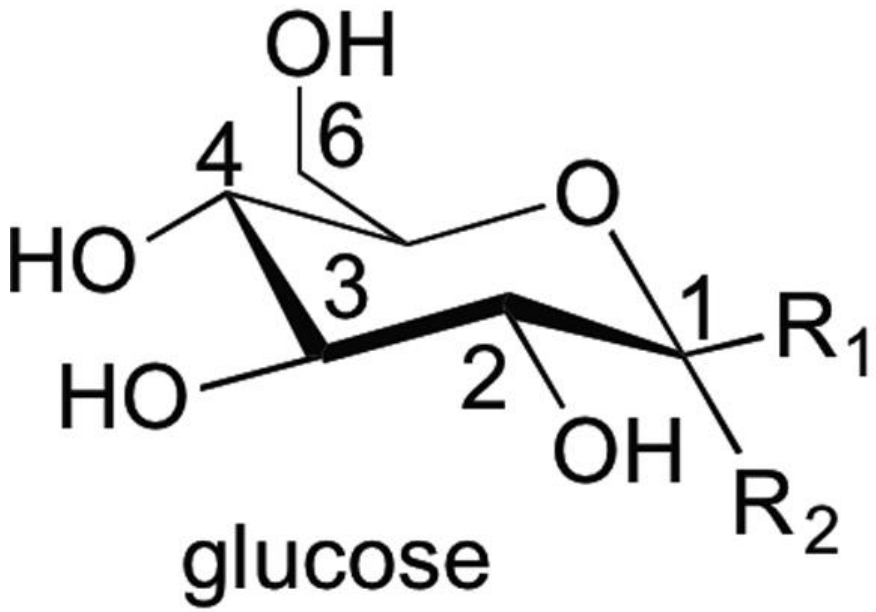
Seoncheol Cha
26 Nov 2016



glucose

α: R_1= H; R_2 = OH

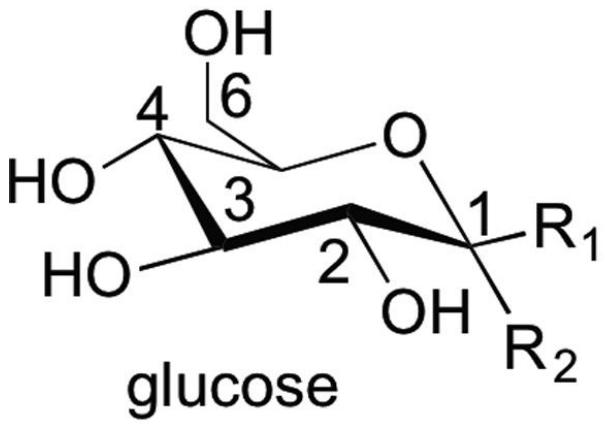
β: R_1= OH; R_2 = H

Exchange Rate of Hydroxyl groups of Glucose aqueous solution : 2000 /s

Reverse Micelle (RM)

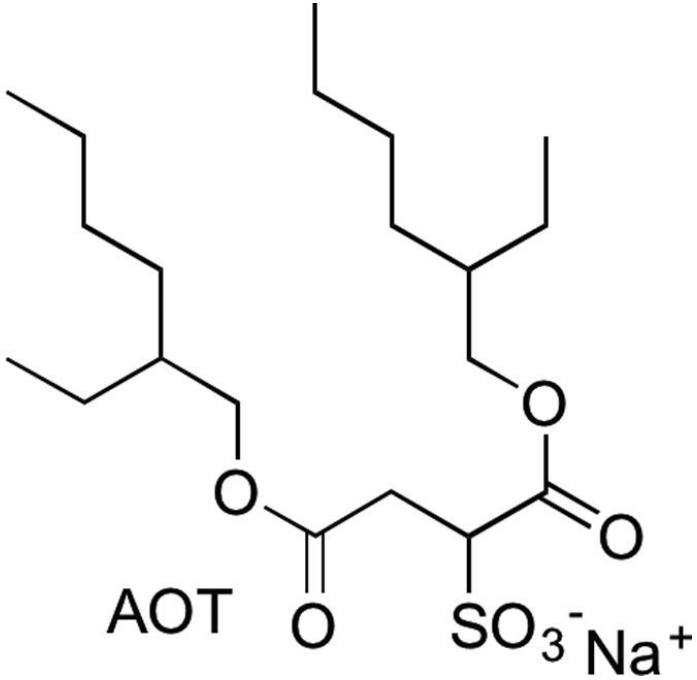
AOT (sodium bis(2-ethylhexyl) sulfosuccinate)

AOT/water
+ 10% cyclohexane-d_{12}/isooctane

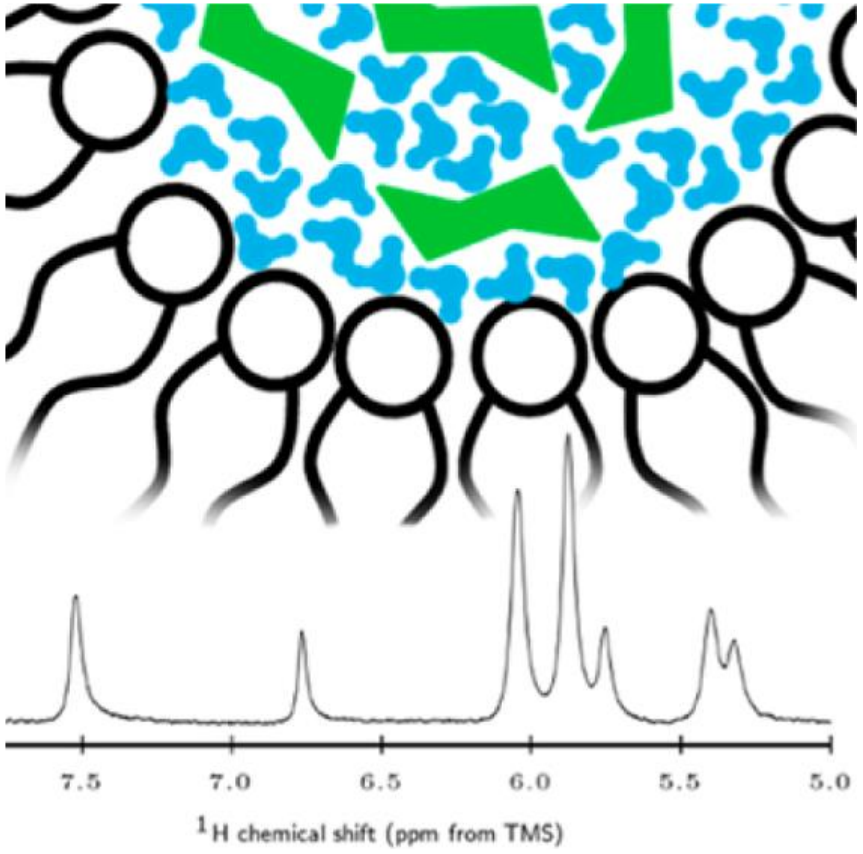


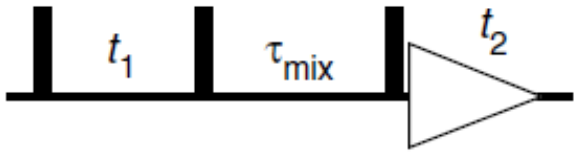
glucose

α: R_1= H; R_2 = OH
β: R_1= OH; R_2 = H



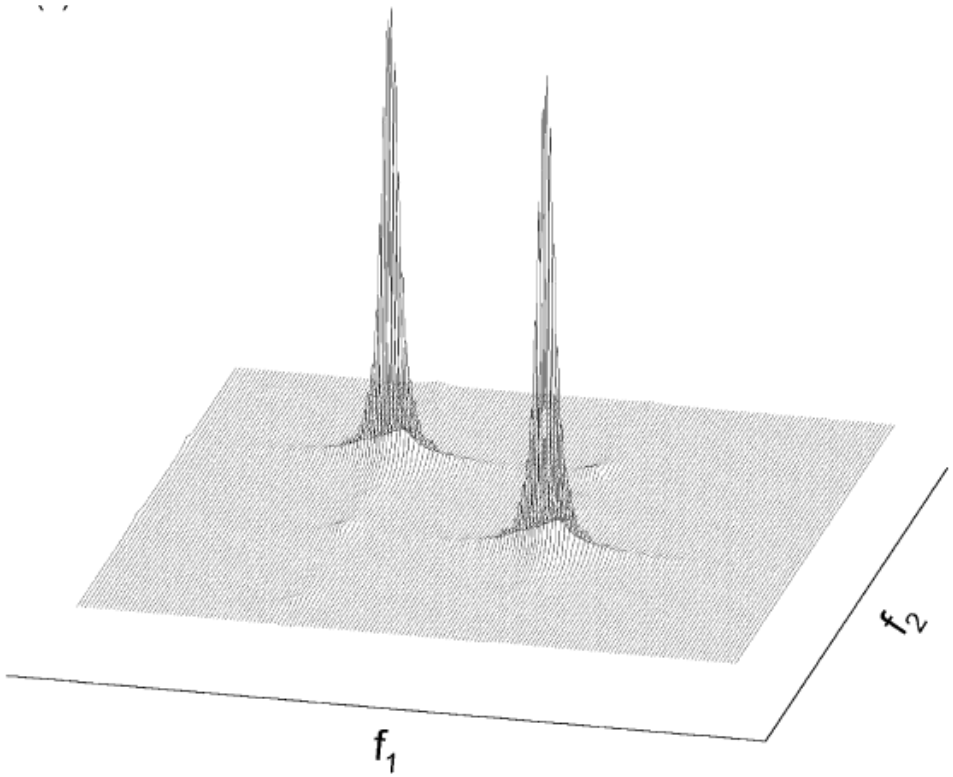
AOT

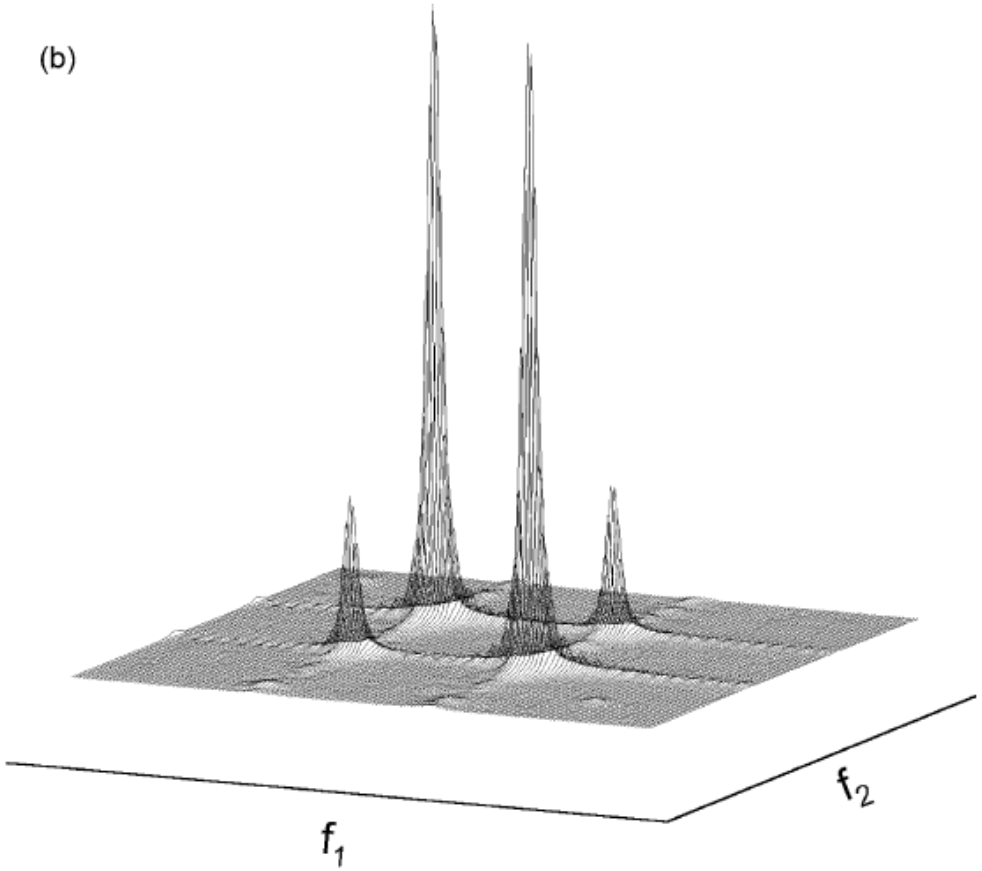




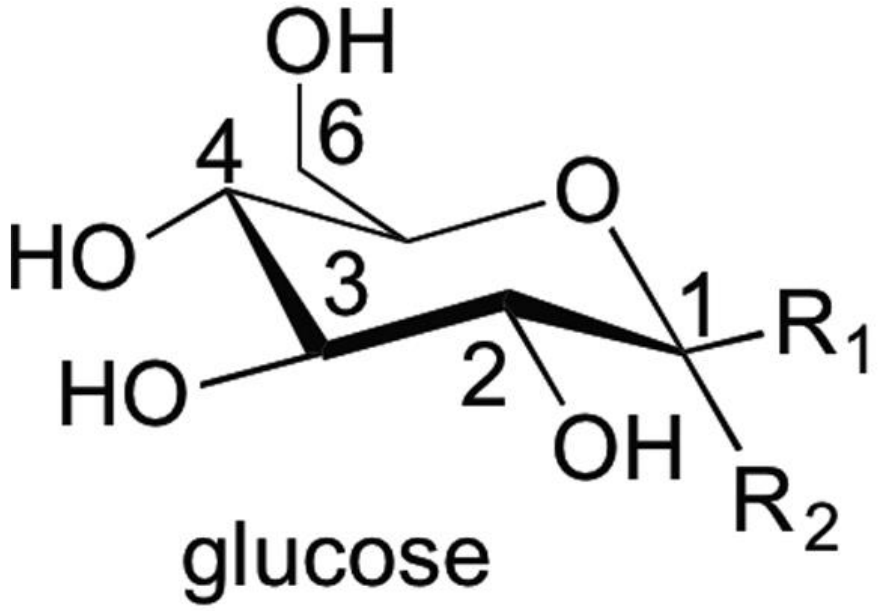
The pulse sequence for EXSY (and NOESY). All pulses have 90° flip angles.

First, the 90° – t_1 – 90° sequence is used to generate frequency labelled z–magnetization. Then, during τ_{mix}, this magnetization is allowed to migrate to other spins, carrying its label with it. Finally, the last pulse renders the z–magnetization observable.

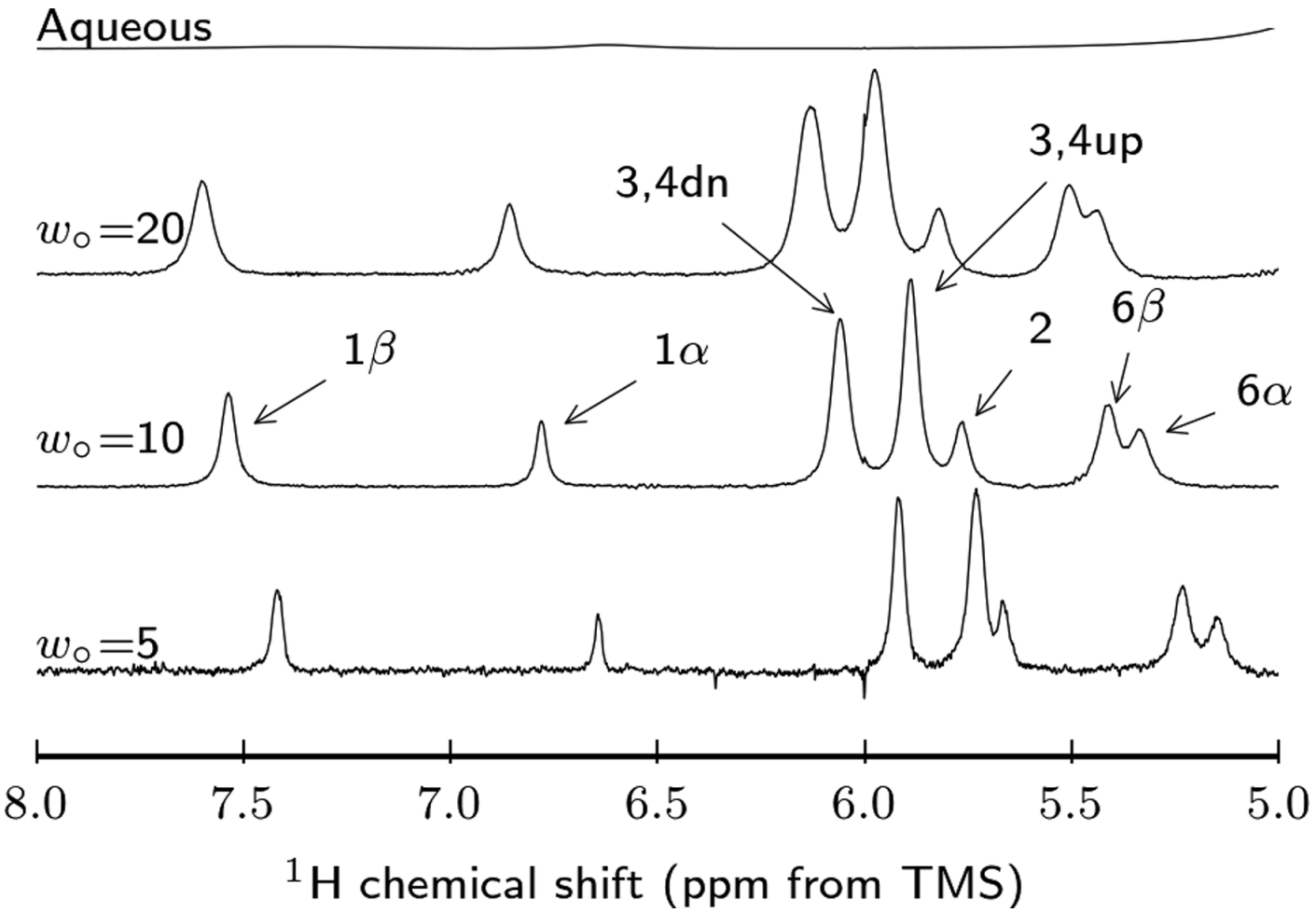


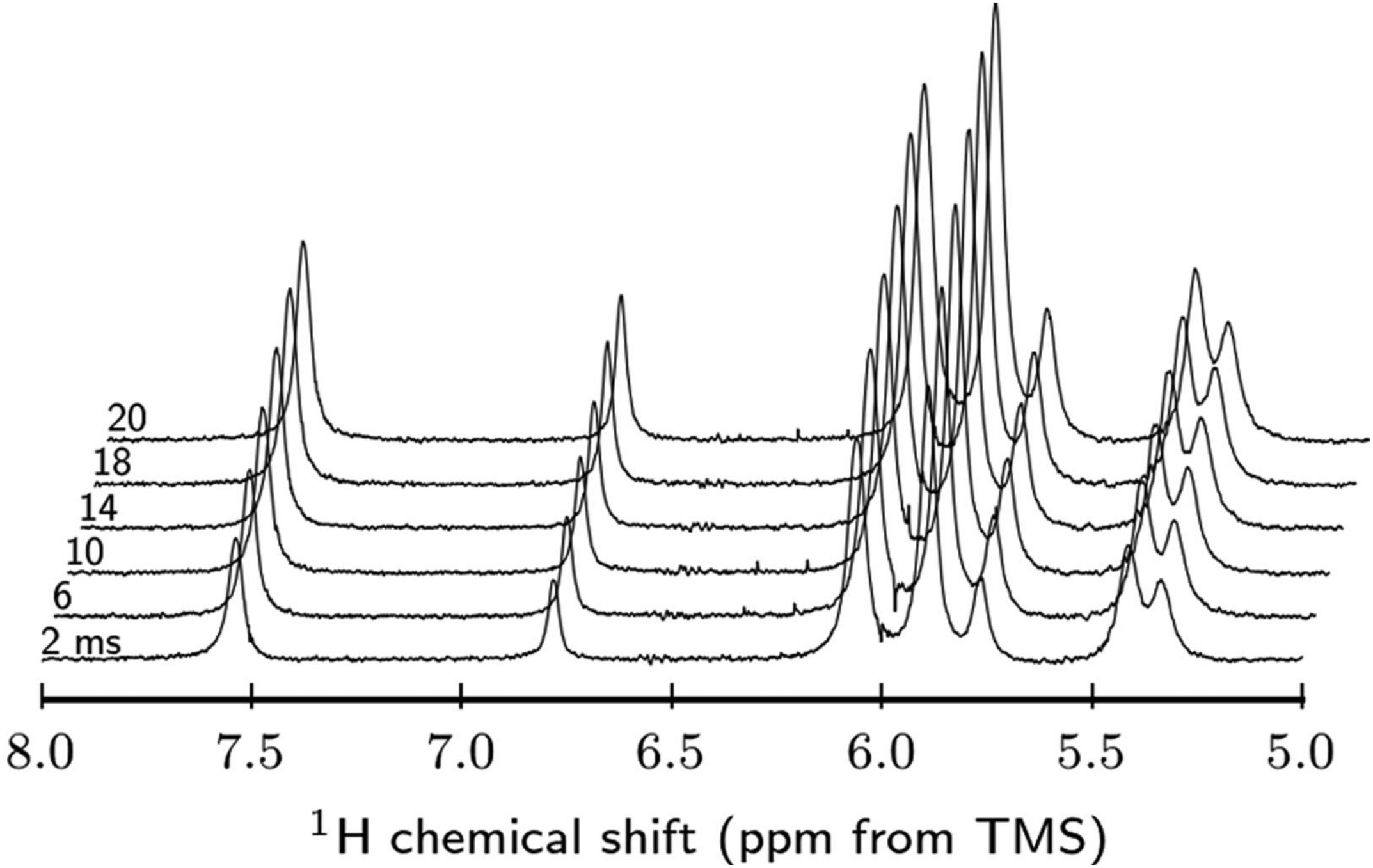


Exchange Rate of glucose bulk : 2000 /s
Exchange Rate of glucose RM < 400 /s



α: R_1= H; R_2 = OH
β: R_1= OH; R_2 = H




20
18
14
10
6
2 ms
8.0
7.5
7.0
6.5
6.0
5.5
5.0
^{1}H chemical shift (ppm from TMS)

$$\mathrm{HOH^*} + \mathrm{GOH} \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} \mathrm{HOH} + \mathrm{GOH^*} \xrightarrow{k_2} \mathrm{HOH} + \mathrm{GOH}$$

$$\mathrm{HOH^*} + \mathrm{GOH} \xrightarrow{k_1} \mathrm{HOH} + \mathrm{GOH^*} \xrightarrow{k_2} \mathrm{HOH} + \mathrm{GOH}$$

$$[\mathrm{GOH^*}] = \frac{k_1}{k_2 - k_1}[\mathrm{GOH}]_0 (\mathrm{e}^{-k_1 t} - \mathrm{e}^{-k_2 t}) + C$$

$$[\mathrm{GOH}^*] = \frac{k_1}{k_2 - k_1}[\mathrm{GOH}]_0(\mathrm{e}^{-k_1 t} - \mathrm{e}^{-k_2 t}) + C$$