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# **Supporting Information**

## Water absorption by deep eutectic solvents

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Figure S1. Fitting curve of the difference IR absorbance of ChCl:xylitol at 3350 cm<sup>-1</sup> and the time for one region. The horizontal axis is the time/min, the vertical axis is A, the absorbance in difference spectra. The fitted equation is  $A=A_{max}(1-e^{-kt})$ , as suggested by Al-Abadleh.<sup>1-3</sup> The  $k_A$ value deriving from this model is 5.02 h<sup>-1</sup>, about five times of the k value (1.04 h<sup>-1</sup>) derived from the water absorption capacity mode  $W=W_{\infty}(1-e^{-kt})$ . It means that the water absorption rate expressed by IR absorbance is higher than that expressed by capacity. It could also be corroborated by the time needed to reach equilibrium: ca. 1.5 hours for the IR absorbance while ca. 4 hours for water absorption capacity. It is because that the ATR-IR only detects the area of several micrometers at the bottom of ChCl:xylitol sample, while the mass gain detects the whole ChCl:xylitol sample. Namely, the bottom area is first saturated by water, and then followed by the whole area of DESs, thus a faster water absorption rate for the former condition. The values of parameters derived from  $A=A_{max}(1-e^{-kt})$  and  $W=W_{\infty}(1-e^{-kt})$  are not consistent, therefore, we select the mass gain-related parameters to express the kinetics due to a more real characterization. However, we can also use the IR spectra to investigate the mechanism owing to the same tendency for them. Also, the three-region model as described below is also consistent with that from PCMW2D-COS spectra.



**Figure S2.** Fitting curve of the difference IR absorbance of ChCI:xylitol at 3350 cm<sup>-1</sup> and the time for three regions. The horizontal axis is the time/min, the vertical axis is the  $ln(1-A/A_{max})$ , where A and  $A_{max}$  means the absorbance in difference spectra and the corresponding maximum absorbance during 240 min, respectively. The fitted equation is  $ln(1-A/A_{max})=kt$ , as suggested by Al-Abadleh.<sup>1</sup> The first region is from 0 min to 35 min; the second region is from 40 min to 100 min, and the third region is from 105 to 240 min, which corresponds to the three regions derived from PCMW-2D-COS spectra from Figure 4.The value of k derived from the water absorption capacity vs time for ChCI:xylitol is 1.04 h<sup>-1</sup>, between the values of  $k_1=2.65$  h<sup>-1</sup> and  $k_2=0.41$  h<sup>-1</sup>,  $k_3=0.03$  h<sup>-1</sup> derived from here by the IR absorbance vs time. It indicates the favorable consistent between the parameters derived from water absorption capacity model and from IR absorbance model. It also means the three-region mechanism from  $ln(1-A/A_{max})=kt$  is better than the oneregion model A=A<sub>max</sub>(1-e<sup>-kt</sup>).



**Figure S3.** Peak deconvolution of difference IR spectra of ChCI:xylitol for OH group over the range  $3040 \sim 3700 \text{ cm}^{-1}$  in the presence of air at 10 min. No baseline correction (up). 2 point baseline correction (down), the red dashed line is the baseline.



**Figure S4.** Peak deconvolution of difference IR spectra of ChCI:xylitol for OH group over the range  $3040 \sim 3700 \text{ cm}^{-1}$  in the presence of air at 240 min. No baseline correction (up). 2 point baseline correction (down), the red dashed line is the baseline.

Table S1. Peak deconvolution of difference IR spectra of ChCI:xylitol for OH group over the range  $3040 \sim 3700 \text{ cm}^{-1}$  in the presence of air at 10 min and 240 min.<sup>a</sup>

#### No baseline correction

	10 min	240 min	10 min	240 min	10 min	240 min	10 min	240 min
	center	center	Absolute	Absolute	Relative	Relative	Width	Width
			Area	Area	Area	Area		
H-O-H…OH <sub>a</sub>	3501.4	3498.5→	3.5	5.4	11.8%	11.4%	42.1	52.2
H-O-H…OH <sub>b</sub>	3410.7	3407.9→	7.4	13.0	24.6%	27.5% †	42.1	52.2
H-O-H…OH <sub>c</sub>	3325.9	3318.5→	8.2	14.2	27.4%	30.0% †	42.1	52.2
H-O-H…OH <sub>d</sub>	3230.2	3221.3→	7.2	11.3	23.9%	23.8%	42.1	52.2
ОН…Н-О-Н…ОН	3137.0	3114.8→	3.7	3.4	12.4%	7.3% 🖌	42.1	52.2
Overall			30.1	47.4	100%	100%		

 $^{\rm a}$   $\rightarrow$  means red shift.  $\uparrow$  and  $\downarrow$  mean increase and decrease, respectively.

After 2 point baseline correction

	10 min	240 min	10 min	240 min	10 min	240 min	10 min	240 min
	center	center	Absolute	Absolute	Relative	Relative	Width	Width
			Area	Area	Area	Area		
H-O-H…OH <sub>a</sub>	3501.4	3498.5→	2.9	4.9	11.0%	11.5%	42.1	52.2
H-O-H…OH <sub>b</sub>	3410.7	3407.9→	6.9	12.3	26.4%	28.6% †	42.1	52.2
H-O-H…OH <sub>c</sub>	3325.9	3318.5→	7.5	13.7	28.6%	31.9% †	42.1	52.2
H-O-H…OH <sub>d</sub>	3230.2	3221.3→	6.5	10.2	24.6%	23.6%	42.1	52.2
ОН…Н-О-Н…ОН	3138.3	3123.3→	2.5	1.9	9.5%	4.4% 🖌	42.1	52.2
Overall			26.2	43.0	100%	100%		

 $^{\rm a}$   $\rightarrow$  means red shift.  $\uparrow$  and  $\downarrow$  mean increase and decrease, respectively.



**Figure S5.** Peak deconvolution of difference IR spectra of ChCl:glucose for OH group over the range  $3000 \sim 3800$  cm<sup>-1</sup> in the presence of air at 10 min. No baseline correction (up). 2 point baseline correction (down), the red dashed line is the baseline.



**Figure S6.** Peak deconvolution of difference IR spectra of ChCl:glucose for OH group over the range  $3000 \sim 3800$  cm<sup>-1</sup> in the presence of air at 240 min. No baseline correction (up). 2 point baseline correction (down), the red dashed line is the baseline.

Table S2. Peak deconvolution of difference IR spectra of ChCl:glucose for OH group over the range 3000 $\sim$ 3800 cm^-1 in the presence of air at 10 min and 240 min. <sup>a</sup>

	10 min	240 min	10 min	240 min	10 min	240 min	10 min	240 min
	center	center	Absolute	Absolute	Relative	Relative	Width	Width
			Area	Area	Area	Area		
H-O-H…OH <sub>a</sub>	3525.7	3461.5→	3.3	9.6	12.5%	14.7% †	58.3	63.3
H-O-H…OH <sub>b</sub>	3399.5	3363.8→	6.6	14.1	25.3%	21.6% 🗸	58.3	63.3
H-O-H…OH <sub>c</sub>	3303.2	3288.6→	6.8	16.1	26.2%	24.5% 🖌	58.3	63.3
H-O-H…OH <sub>d</sub>	3215.6	3208.8→	6.1	15.9	23.3%	24.3% †	58.3	63.3
ОН…Н-О-Н…ОН	3126.6	3110.2→	2.4	8.0	9.4%	12.3% †	58.3	63.3
Н-О-Н…О=С-Н	3067.3	3049.9→	0.9	1.7	3.4%	2.5% 🖌	23.9	26.4
Overall			26.1	65.4	100%	100%		

No baseline correction

 $^{\rm a}$   $\rightarrow$  means red shift.  $\uparrow$  and  $\downarrow$  mean increase and decrease, respectively.

#### After 2 point baseline correction

	10 min	240 min	10 min	240 min	10 min	240 min	10 min	240 min
	center	center	Absolute	Absolute	Relative	Relative	Width	Width
			Area	Area	Area	Area		
H-O-H…OH <sub>a</sub>	3525.7	3461.5→	3.3	9.0	12.1%	14.7% †	58.3	63.3
H-O-H…OH <sub>b</sub>	3399.5	3363.8→	6.7	13.1	24.7%	21.4% 🖌	58.3	63.3
H-O-H…OH <sub>c</sub>	3303.2	3288.6→	7.2	15.7	26.5%	25.7% 🗸	58.3	63.3
H-O-H…OH <sub>d</sub>	3215.6	3208.9→	5.9	15.5	22.0%	25.4% †	58.3	63.3
ОН…Н-О-Н…ОН	3128.9	3116.2→	3.0	7.0	11.1%	11.5% †	58.3	63.3
H-O-H…O=C-H	3067.5	3051.9→	1.0	0.9	3.6%	1.4% 🖡	23.9	26.4
Overall			27.0	61.2	100%	100%		

 $^{\rm a}$   $\rightarrow$  means red shift.  $\uparrow$  and  $\downarrow$  mean increase and decrease, respectively.



**Figure S7.** Normalized IR spectra of D<sub>2</sub>O, ChCl:xylitol and the D<sub>2</sub>O+ChCl:xylitol mixture. The mass ratio of D<sub>2</sub>O to ChCl:xylitol was ca. 7 wt. %. The representative IR peak of D<sub>2</sub>O in pure D<sub>2</sub>O (2553.7 cm<sup>-1</sup>) and ChCl:xylitol+D<sub>2</sub>O (2501.6 cm<sup>-1</sup>), showing the red shift of ca. 52 cm<sup>-1</sup> after interacting with ChCl:xylitol. Another evidence of stronger hydrogen-bonding interaction between ChCl:xylitol and D<sub>2</sub>O than between ChCl:glucose and D<sub>2</sub>O was the broader IR band in the range of 3000-3600 cm<sup>-1</sup> for ChCl:xylitol+D<sub>2</sub>O mixture.



**Figure S8.** Normalized IR spectra of D<sub>2</sub>O, ChCl:glucose and the D<sub>2</sub>O+ChCl:glucose mixture. The mass ratio of D<sub>2</sub>O to ChCl:glucose was ca. 7 wt. %. The representative IR peak of D<sub>2</sub>O in pure D<sub>2</sub>O (2553.7 cm<sup>-1</sup>) and ChCl:glucose+D<sub>2</sub>O (2503.5 cm<sup>-1</sup>), showing the red shift of ca. 50 cm<sup>-1</sup> after interacting with ChCl:glucose.

### **References:**

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