Electronic Supplementary Information (ESI)

Structure, molecular dynamics and interactions in aqueous xylitol solutions

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Table S1. Densities, *d*, viscosities, η, and parameters of the 5D model for the dielectric spectra of aqueous xylitol solutions at 25 °C: static permittivity, ε_s, high-frequency permittivity, ε_∞, amplitudes, S_j, and relaxation times, τ_j, of the resolved modes j = 1…5. Bold font indicates fixed parameter values.

c / M	d / g·cm^{-3}	η / mPa·s	ε_s	ε_∞	S_1	τ_1 / ps	S_2	τ_2 / ps	S_3	τ_3 / ps	S_4	τ_4 / ps	S_5	τ_5 / ps
0.100	1.0021	0.913	78.11	**3.52**			1.14	**21.9**	70.99	8.39			2.46	**0.278**
0.200	1.0072	0.951	77.80	**3.52**			2.29	**22.3**	69.53	8.48			2.46	**0.278**
0.400	1.0171	1.029	77.48	**3.52**			4.48	**23.0**	66.65	8.67			2.83	**0.278**
0.800	1.0370	1.23	76.56	**3.52**			8.79	**24.5**	61.07	9.10			3.19	**0.278**
1.206	1.0572	1.48	75.79	**3.52**	0.73	186	12.59	22.8	55.50	9.50			3.46	**0.278**
1.611	1.0767	1.82	74.24	**3.52**	1.44	109	15.61	27.9	48.20	10.6	2.63	**4.0**	2.84	**0.278**
2.011	1.0961	2.25	73.30	**3.52**	2.75	105	19.34	28.7	41.99	11.3	3.17	**3.5**	2.53	**0.278**
2.181	1.1043	2.48	72.85	**3.52**	3.35	99	21.95	28.4	38.06	11.3	3.23	4.46	2.73	**0.278**
2.388	1.1150	2.83	72.22	**3.52**	3.58	111	22.74	30.8	36.27	11.8	3.33	4.36	2.78	**0.278**
2.816	1.1362	3.76	70.98	**3.52**	5.69	112	27.60	31.5	27.70	11.9	3.54	**5.9**	2.92	**0.278**
3.251	1.1579	5.12	69.51	**3.52**	8.48	116	29.54	33.5	21.56	12.5	3.76	**5.2**	2.66	**0.278**

Table S2. Parameters a_i of n^{th} order polynomials, $\Sigma a_i \times c^i$ ($0 \le i \le n$), fitting density, d, static permittivity, ε_s, amplitudes S_2 & S_4 (Table S1), and S_s & S_b (see main text), as well as relaxation times τ_2 and τ_3 (Table S1) as a function of concentration, c, of aqueous xylitol solutions at 298.15 K.[a]

	n	a_0	a_1	a_2
d / kg·L^{-1}	2	0.99727±0.00013	0.04931±0.00008	
ε_s	2	**78.368**[b]	-2.143±0.082	-0.178±0.032
S_2	2	**0**	10.96±0.35	-0.53±0.14
S_4	2	**0**	2.154±0.055	-0.311±0.021
S_s	1	**0**	7.560±0.083	
S_b	1	**74.848**[b]	-15.38±0.10	
τ_2/ps	1	21.6±1.24	3.61±0.51	
τ_3/ps	1	**8.35**[b]	1.310±0.040	

[a] $S_1 = (0.471 \pm 0.059) \times c^{(2.44 \pm 0.12)}$ with c in M; [b] ref [1]; bold font indicates fixed parameter.

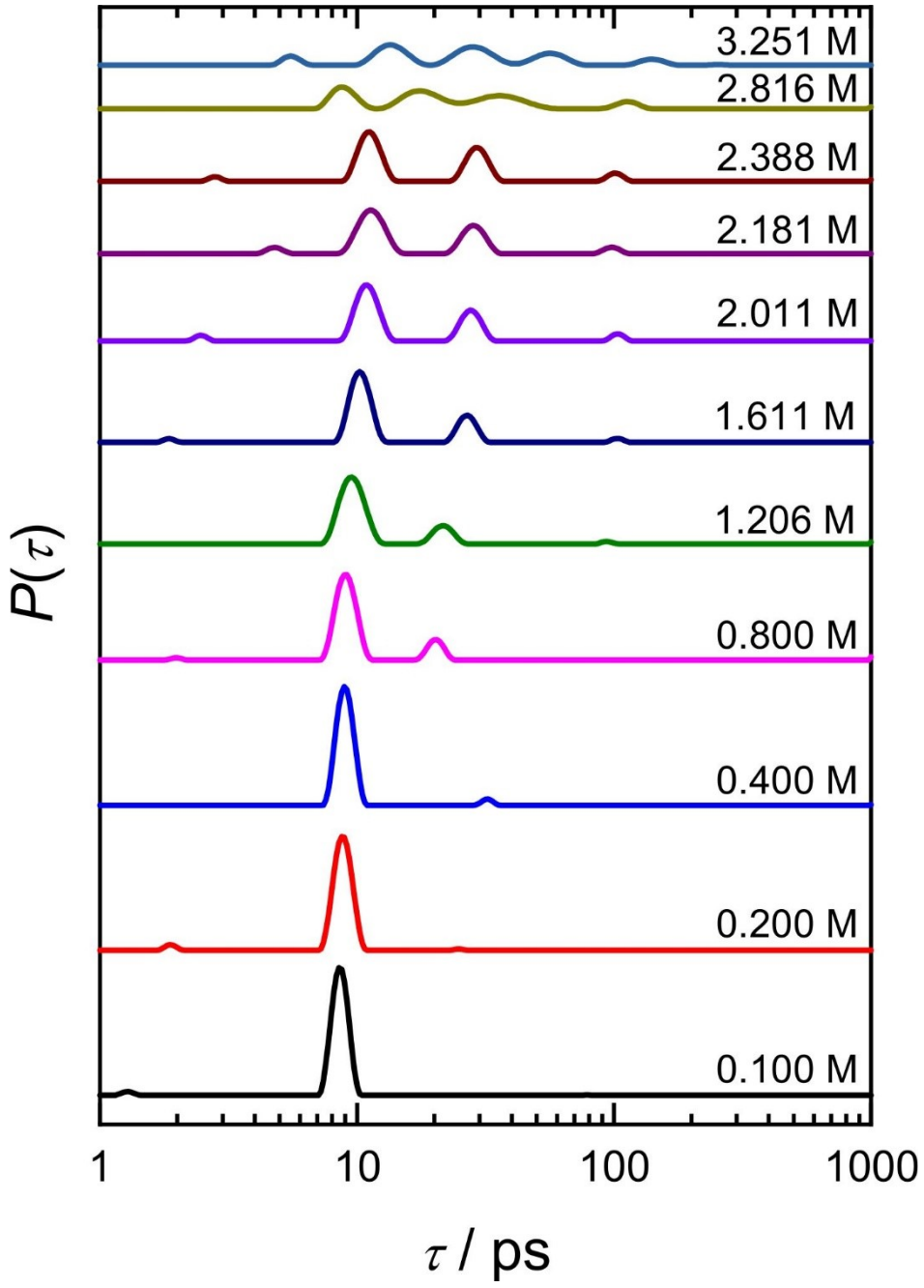

Fig. S1. Relaxation-time probability functions, $P(\tau)$,[2] for the investigated aqueous xylitol solutions at 25 °C.

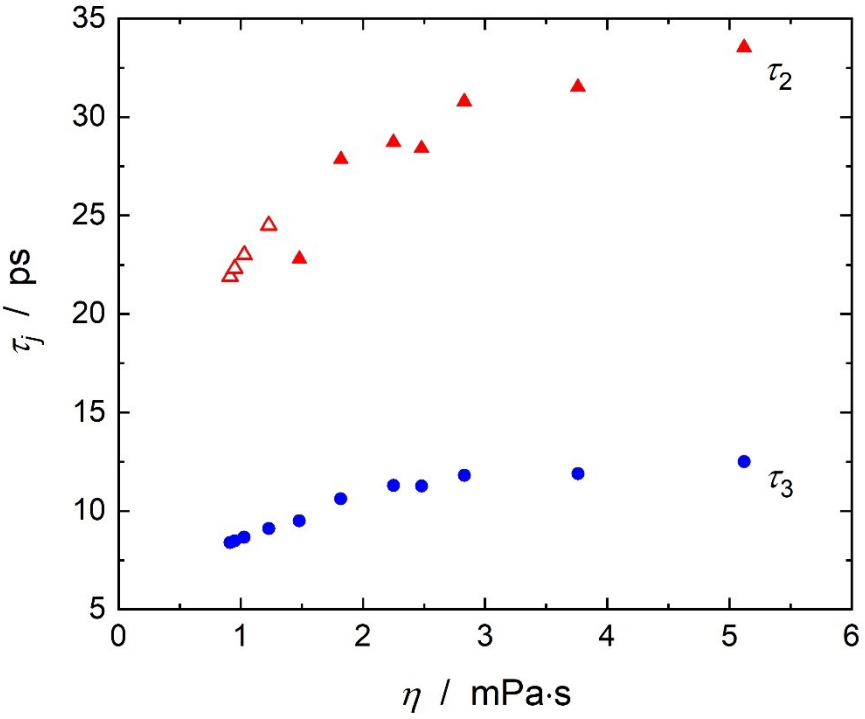

Fig. S2. Water-related relaxation times, τ_2 (▲) and τ_3 (●), as a function of solution viscosity, η, for aqueous xylitol solutions at 298.15 K.

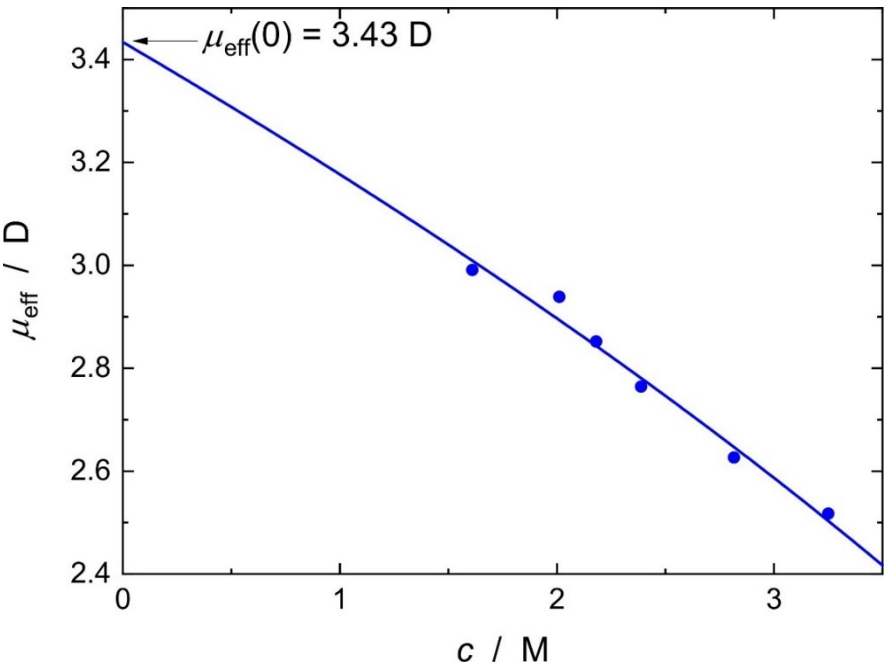

Fig. S3. Effective dipole moment, μ_{eff} (●), of an OH group of xylitol calculated from the amplitude S_4 of Table S1. The line was obtained with the polynomial fitting S_4 (Table S2).

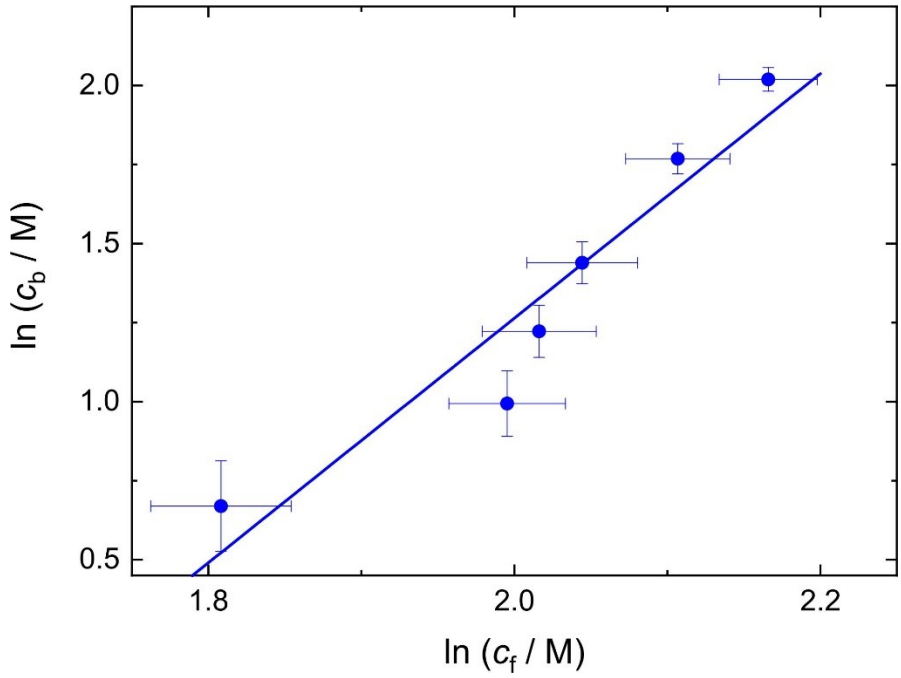

Fig. S4. Concentration of bound xylitol hydroxy groups, c_b (●), as a function of the concentration of free xylitol hydroxy groups, c_f, and associated fit with eqn. 3 (line).

Notes and references

1. A. Eiberweiser, A. Nazet, G. Hefter, and R. Buchner, *J. Phys. Chem. B*, 2015, **119**, 5270-5281.
2. A. Y. Zasetzky and R. Buchner, *J. Phys.: Condens. Matter*, 2011, **23**, 025903.