Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

A study of the interaction between TMAO and urea in water using NMR spectroscopy.

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Supplementary Information

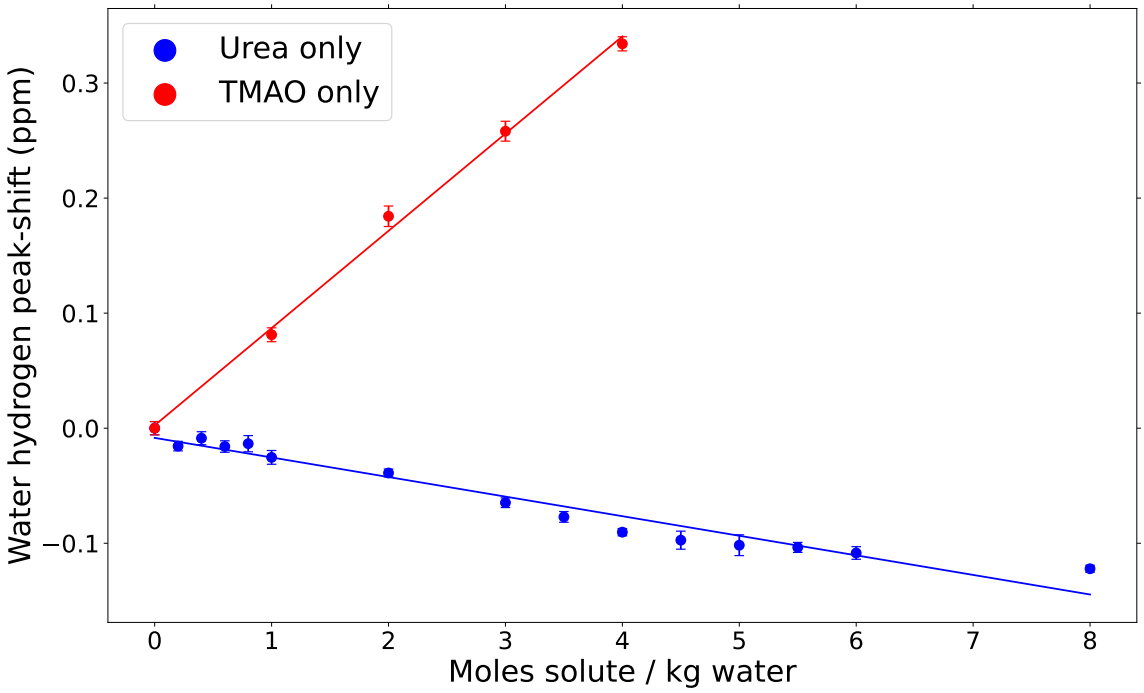

Figure S1: The NMR spectral peaks of hydrogen atoms in binary solutions of aqueous urea and TMAO reveal opposing effects. TMAO generates a strong blue shift in the spectral peak of hydrogen atoms in water indicative of strong hydrogen bonding, whilst urea generates a relatively minor effect. The lines are linear fits to the data points.

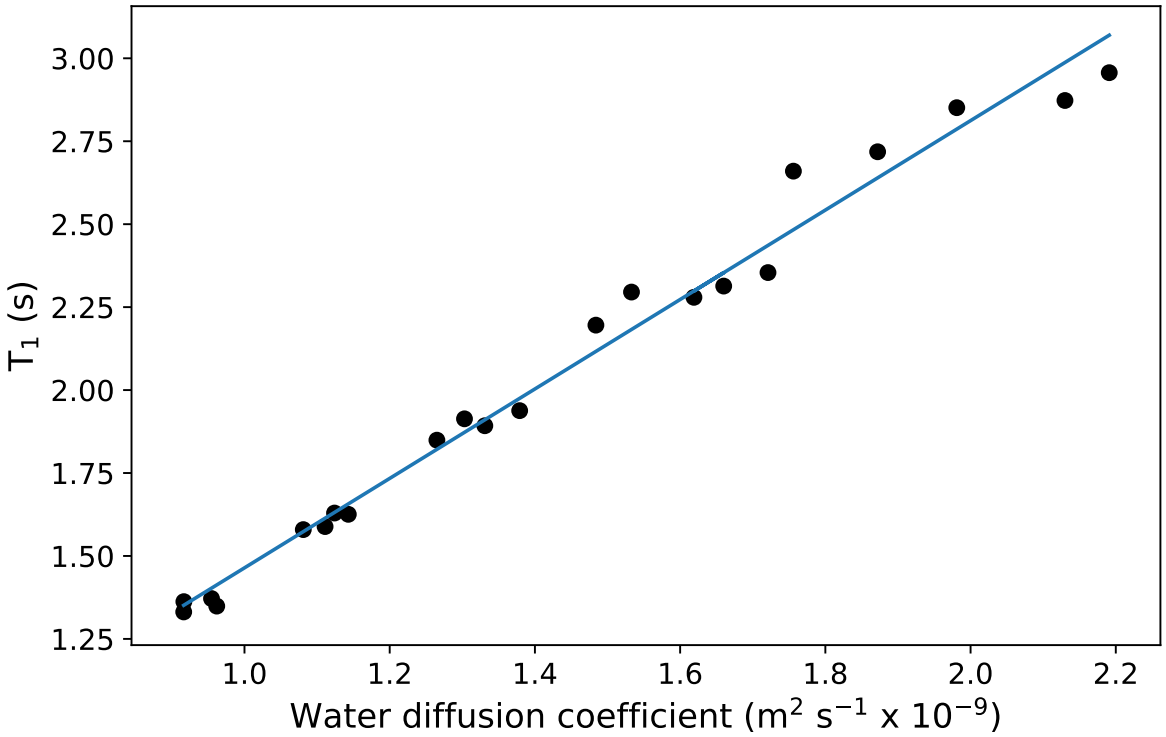

Figure S2: A comparison of the diffusion coefficient and T_1 for water in TMAO-urea-water mixtures. The correlation implies that the data is self-consistent and that the translational and rotational dynamics are driven by the same micro-viscosity.

Table 1: The H^1 peak-shifts in TMAO and urea were measured in 16 mixed TMAO-urea-water solutions at 300 K. The experiment was repeated three times and the values recorded below are the mean measurements. The peak-shift in TMAO was benchmarked to 1 molal TMAO in pure water, whilst the peak-shift in Urea was bench-marked to an 8 molal urea solution.

TMAO (Molal)	Urea (Molal)	H^1 TMAO peak-shift (ppm)	H^1 urea peak-shift (ppm)
1.0	1.9	-0.011	0.053
1.0	3.9	-0.021	0.052
1.0	5.8	-0.026	0.047
1.0	7.7	-0.037	0.039
1.9	1.9	0.005	0.095
1.9	3.9	-0.004	0.09
1.9	5.8	-0.016	0.081
1.9	7.7	-0.027	0.078
2.7	1.9	0.015	0.131
2.7	3.9	0.004	0.12
2.7	5.8	-0.011	0.112
2.7	7.7	-0.008	0.119
3.5	1.9	0.014	0.155
3.5	3.9	0.006	0.149
3.5	5.8	-0.004	0.143
3.5	7.7	0.000	0.148