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

Prediction of the concentration dependence of the surface tension and density of salt solutions: atomistic simulations with Drude oscillator polarizable and nonpolarizable models.

1 Nonpolarizable water models

Two nonpolarizable models for water are considered: the SPC/E[1] and TIP4P/2005[2] models. The SPC/E model represents the water molecules as rigid molecules with three point masses with OH distance of 1 Å and HOH angle equal to the tetrahedral angle. The TIP4P/2005 water model[2] is a rigid four-point model with three points charges and one Lennard-Jones interaction site located at the oxygen atom. The Lennard-Jones parameters and the partial charges are given in Table S1 for these two models.

Table S1 The Lennard-Jones well depth ε and size σ, partial charges q for the two nonpolarizable water models, k_B is the Boltzmann's constant.

	SPC/E model[1]		
	σ (Å)	ε/k_B (K)	q ($\|e\|$)
O	3.166	78.205	-0.8476
H	0	0	0.4238
OH distance / (Å)	1.0		
H-O-H angle / (deg)	109.47		

	TIP4P/2005 model[2]		
	σ (Å)	ε/k_B (K)	q ($\|e\|$)
O	3.1589	93.2	0
H	0	0	0.5564
M	0	0	-1.1128
OH distance / (Å)	0.9572		
H-O-H angle / (deg)	104.52		
OM distance / (Å)	0.1546		

References

1 H. J. C. Berendsen, J. R. Grigera and T. P. Straatsma, *J. Phys. Chem.*, 1987, **91**, 6269–6271.
2 J. L. F. Abascal and C. Vega, *J. Chem. Phys.*, 2005, **123**, 234505.