Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Structure Simulations for the 0.22 and 1 Molar Aqueous Dimethylammonium Chloride Solutions

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Supplementary Information

Table S1. IEF-PCM/B3LYP/6-311++G** optimized geometry and derived charges for the $CH_3NH_2CH_3^+$ solute in aqueous solution using different cavity models

Geometry	Bondi/united methyl	UA0	Bondi/all-atom
N-H_{av}	1.023	1.037	1.022
N-C_{av}	1.500	1.499	1.498
C-H_{av}	1.089	1.089	1.087
HNH	105.47	104.69	105.56
HNC_{av}	109.32	109.61	109.22
CNC	113.77	113.67	114.06
HCN_{av}	108.38	108.52	108.40
Charges[a]	CHELPG	CHELPG	CHELPG
N	0.043	0.015	0.058
H(N)	0.290	0.310	0.284
C	-0.251	-0.245	-0.232
H(C)	0.147	0.143	0.140

For Bondi/united methyl, radii from ref. 14b. In the Bondi/all-atom model, the carbon and methyl-hydrogen radii were set to 1.7 (the radius for a carbon atom in ref.14b) and 1.2 Å, respectively, and a scaling factor 1.2 was applied, whereas the N and polar H parameters were preserved as used in the Bondi/united methyl optimization. The number of cavity centers are 5, 3 (UA0) and 11 through the geometry optimizations with the three cavity models, respectively. [a]Rounded charges.

Table S2. Geometric parameters obtained in IEF-PCM/6-311++G** optimizations for the complexes in aqueous solution

$CH_3NH_2^+CH_3\ldots Cl^-$	MP2	B97D
N-H(…Cl)	1.056	1.065
H…Cl^-	1.967	2.020
N…Cl^-	3.013	3.080
N-H…Cl^-	170.1	173.3
$CH_3NH_2^+CH_3\ldots OH_2$		
N-H(…O)	1.040	1.053
H…O	1.749	1.733
N…O	2.776	2.781
N-H…O	168.6	173.1

Bond lengths in Å, bond angles in degrees. Geometric data for the dimethylammonium hydrogen in hydrogen bond to the partner molecule in the complex.

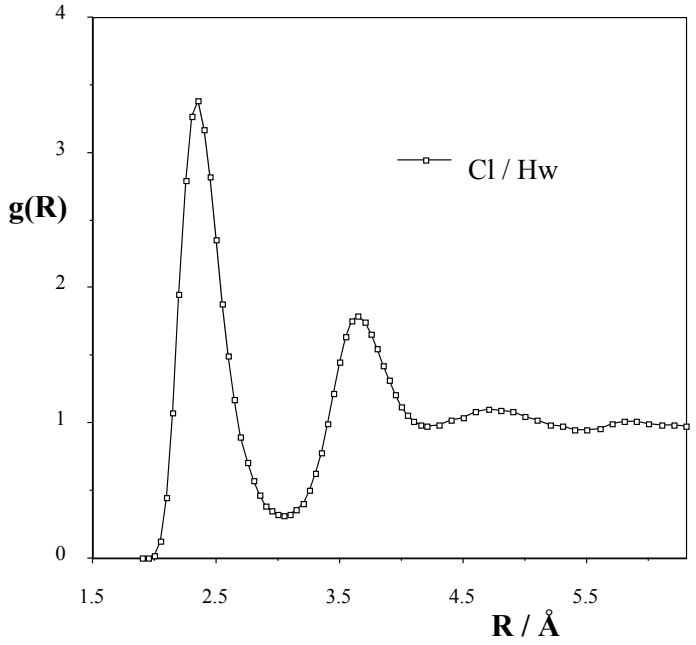

Fig. S1. A $Cl^-\ldots H_{water}$ radial distribution function when the anion is fully exposed to solvation. First maximum and minimum are at R = 2.35 Å and 3.05 Å, respectively. Assuming a linear $O\text{-}H_1\ldots Cl^-$ hydrogen bond of 2.35 Å with a TIP4P water molecule, the $Cl^-\ldots H_2$ distance (distance to the other hydrogen) is 3.67 Å, accounting for the second peak.