Supplementary Material

Molecular Insights into the Urea-Choline-*O*-sulfate Interactions in Aqueous Solution

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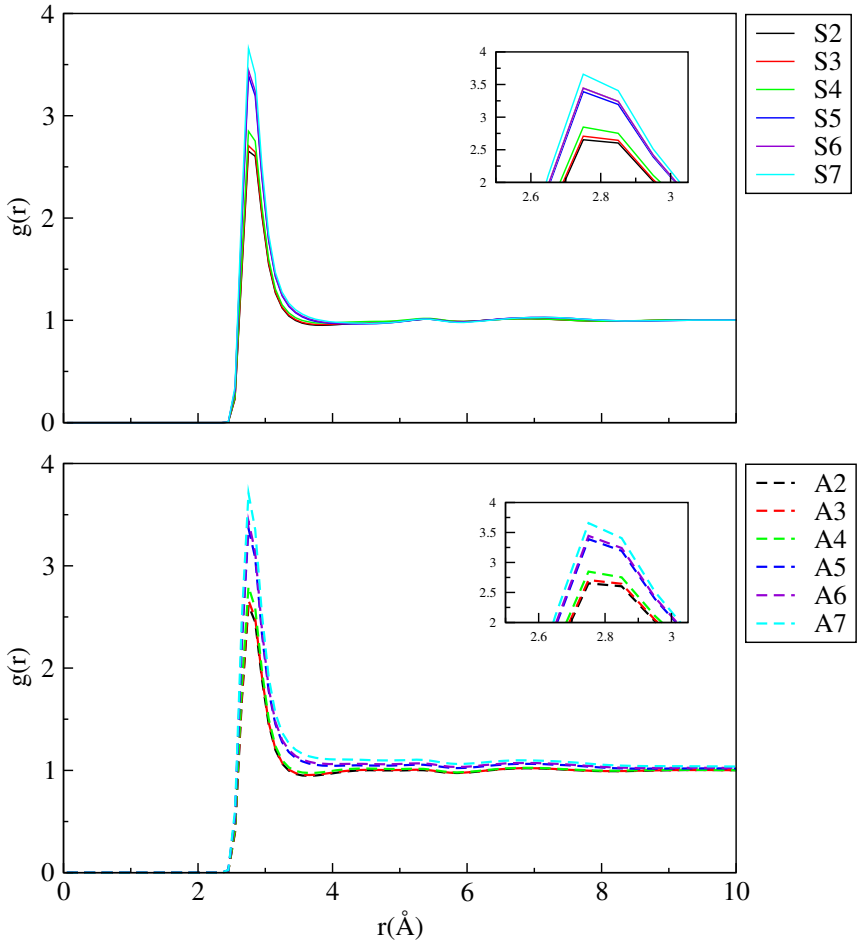

FIG. S1: O_W-O_W rdf plots for 0.3 M COS (systems S2 and A2), 0.5 M COS (systems S3 and A3), 1.0 M COS (systems S4 and A4) and 0.3 M COS + urea (systems S5 and A5), 0.5 M COS + urea (systems S6 and A6) and 1.0 M COS + urea (systems S7 and A7) for CHARMM and GAFF parameters.

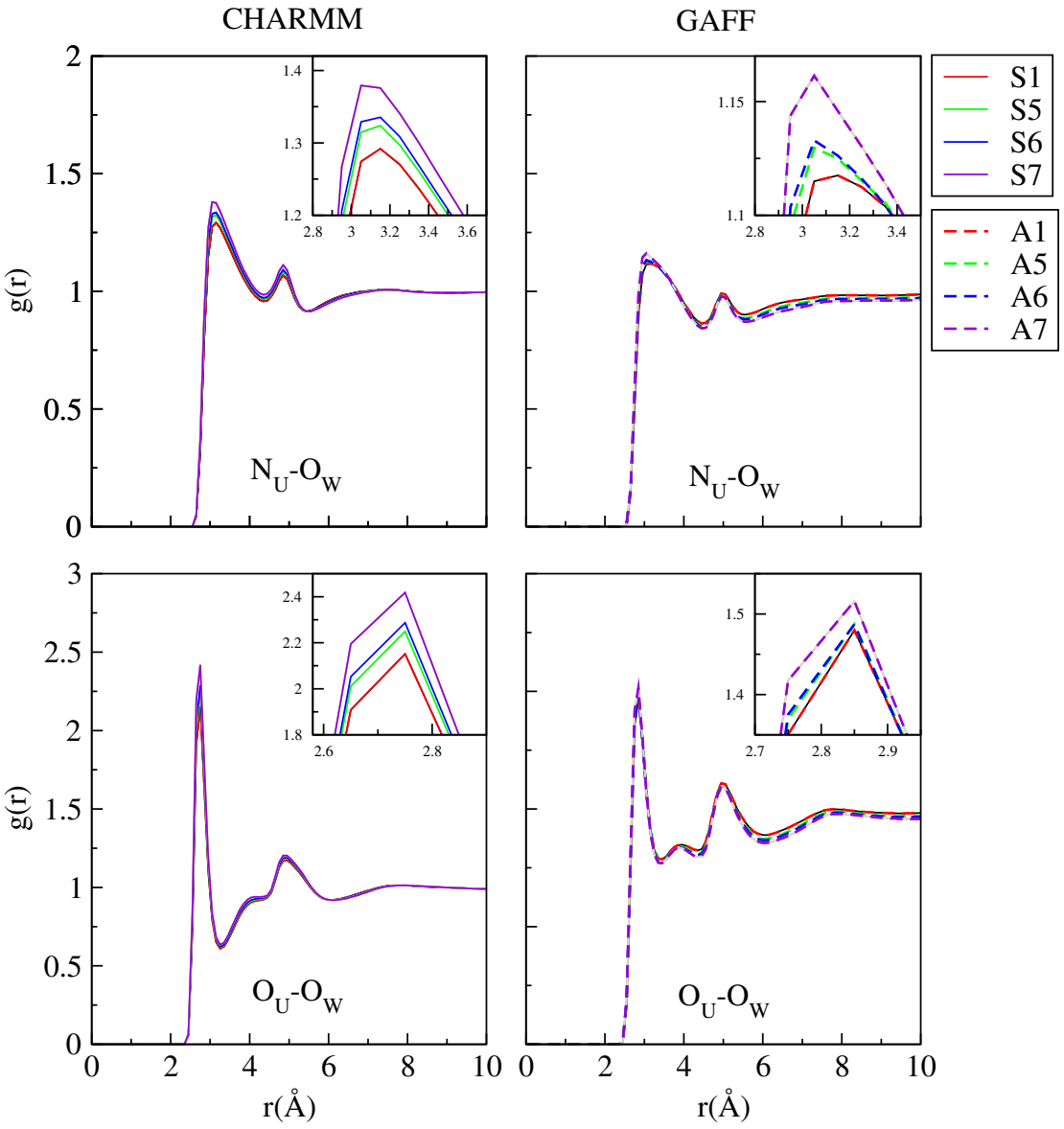

FIG. S2: Urea-water (N_U-O_W and O_U-O_W) rdf plots for 8.0 M urea systems (S1 and A1), 0.3 M COS + urea systems (S5 and A5), 0.5 M COS + urea systems (S6 and A6) and 1.0 M COS + urea systems (S7 and A7). The left and right panels denotes the systems with CHARMM and GAFF parameters respectively.

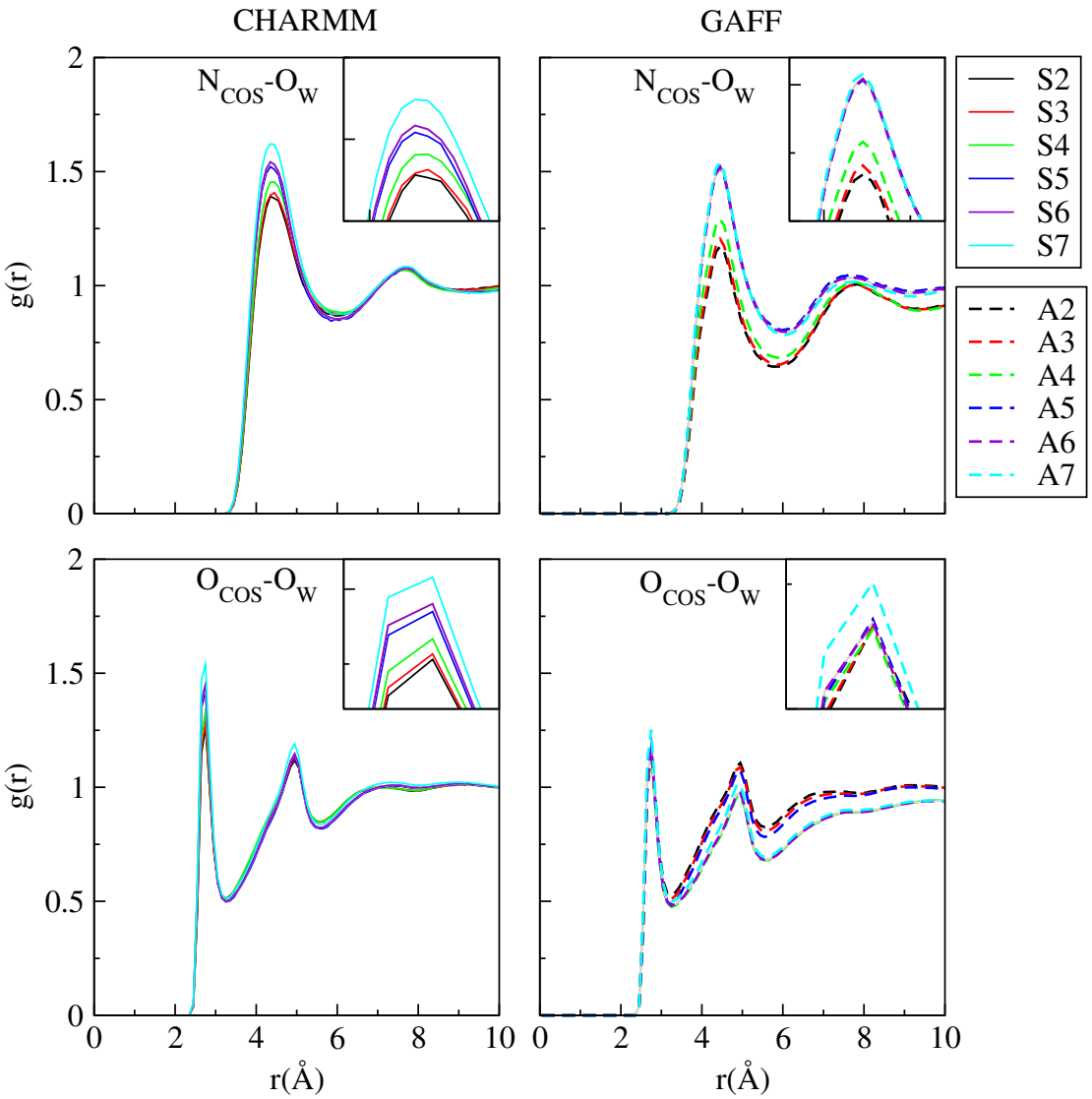

FIG. S3: Radial distribution functions of N_{COS}-O_W and O_{COS}-O_W for 0.3 M COS (system S2 ans A2), 0.5 M COS (systems S3 and A3), 1.0 M COS (systems S4 and A4) and 0.3 M COS + urea (systems S5 and A5), 0.5 M COS + urea (systems S6 and A6), 1.0 M COS + urea (systems S7 and A7). Left panel is for CHARMM parameter systems and right panel is for GAFF parameter systems.

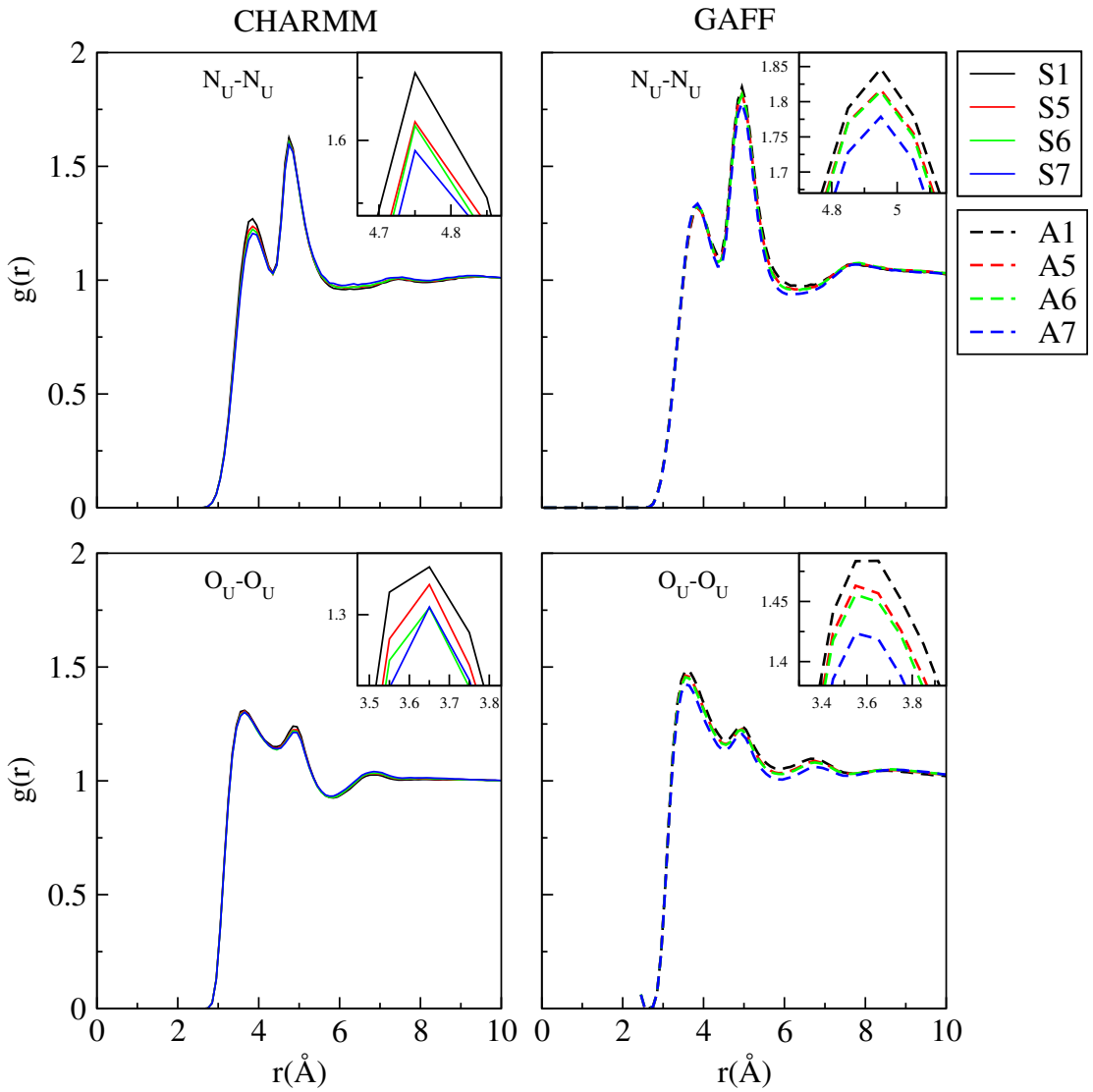

FIG. S4: Radial distribution functions of N_U-N_U and O_U-O_U for 8.0 M urea solution (systems S1 and A1) and 0.3 M COS + urea (systems S5 and A5), 0.5 M COS + urea (systems S6 and A6), 1.0 M COS + urea (systems S7 and A7). Left panel is for CHARMM parameter systems and right panel is for GAFF parameter systems.

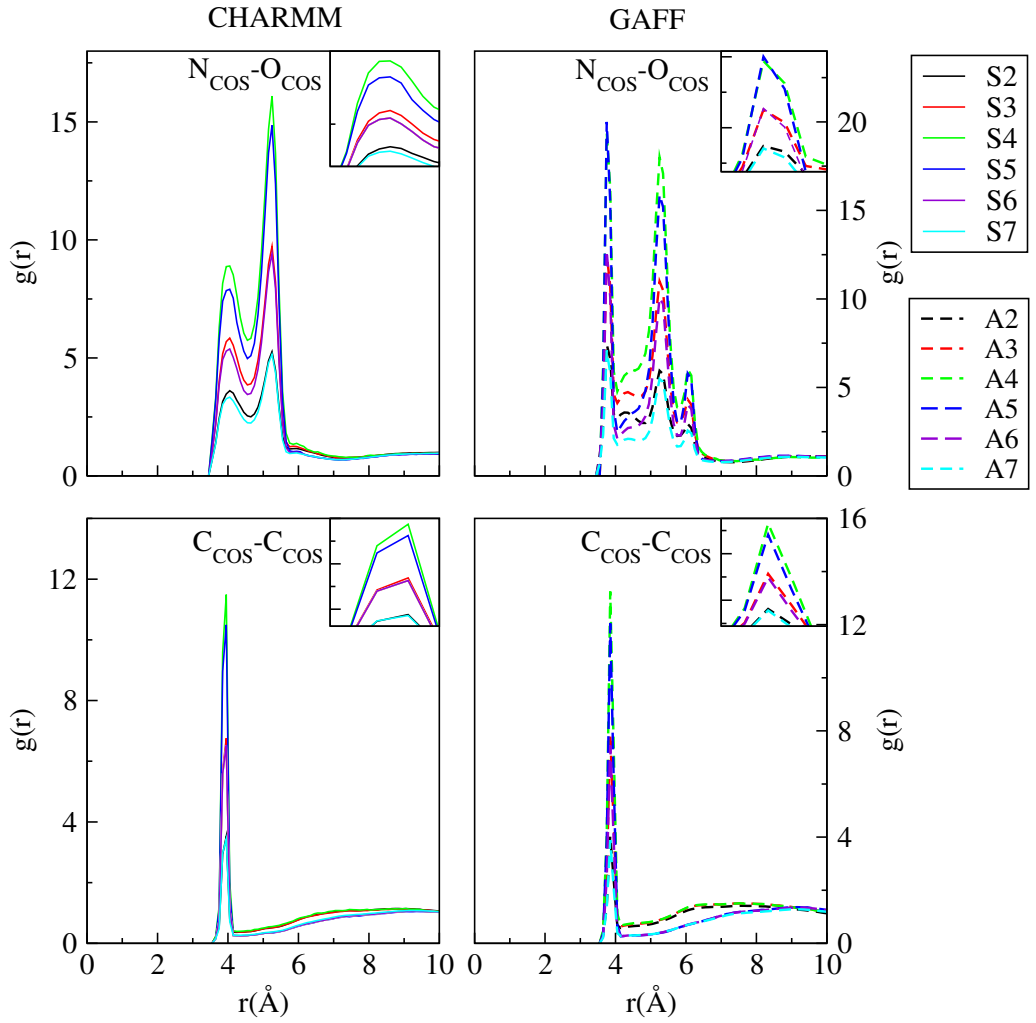

FIG. S5: Radial distribution functions of N_{COS}-O_{COS} and C_{COS}-C_{COS} for O.3 M COS (systems S2 and A2), 0.5 M COS (systems S3 and A3), 1.0 M COS (systems S4 and A4) and 0.3 M COS + urea (systems S5 and A5), 0.5 M COS + urea (systems S6 and A6), 1.0 M COS + urea (systems S7 and A7). Left panel is for CHARMM parameter systems and right panel is for GAFF parameter systems.

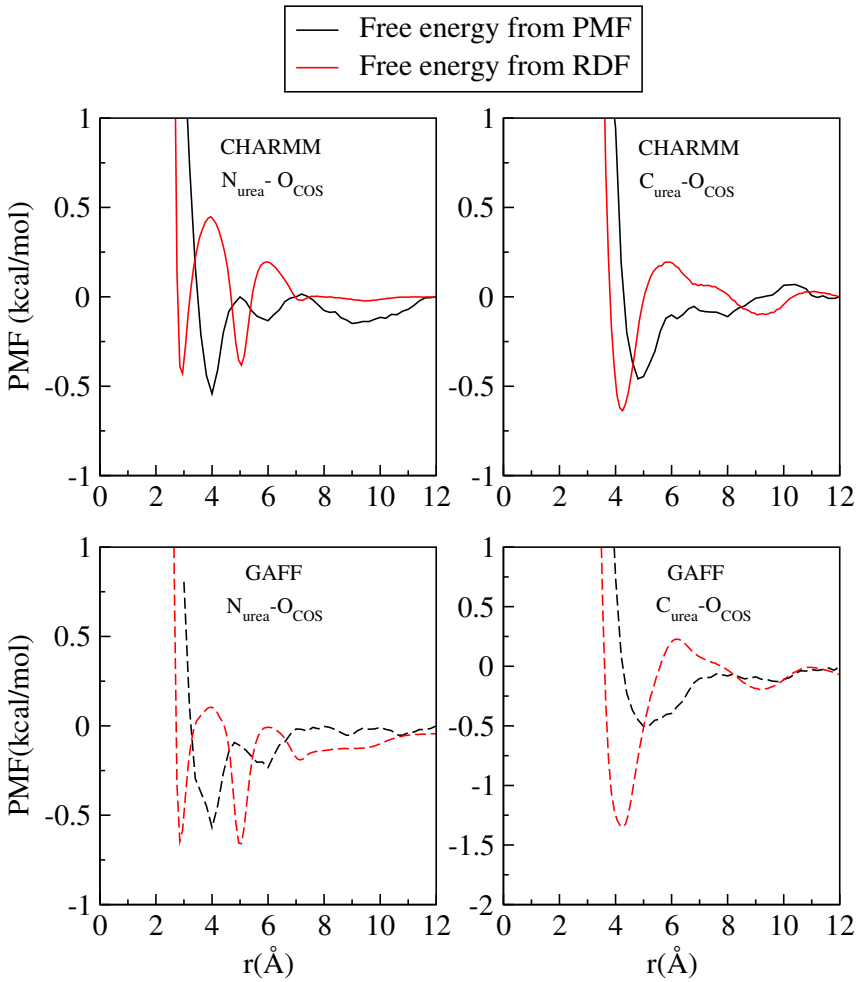

FIG. S6: Free energy of seperation between N_{urea} and O_{COS} and C_{urea} and N_{COS} for systems with 1.0 M COS + urea at 310 K (systems S7 and A7). Upper panel is for CHARMM parameter systems and lower panel is for GAFF parameter systems.

System	cn-urea-water	System	cn-urea-water
S1	9.10 (5.82)	A1	8.47 (5.53)
S5	8.27 (4.80)	A5	7.60 (4.50)
S6	8.22 (4.68)	A6	7.52 (4.37)
S7	7.47 (3.81)	A7	6.80 (3.54)
S7a	7.36 (3.61)	A7a	6.37 (3.36)

TABLE S1: Coordination number of water around urea. The normalised values with respect to the density of water in the pure water system are given in the parenthesis.

System	cn-COS-water	System	cn-COS-water
S2	32.52 (31.54)	A2	31.51 (30.22)
S3	31.20 (29.02)	A3	30.01 (26.76)
S4	28.57 (24.85)	A4	26.73 (23.45)
S5	21.60 (12.53)	A5	17.88 (10.58)
S6	21.10 (12.03)	A6	17.44 (10.14)
S7	18.97 (9.67)	A7	15.91 (8.28)
S7a	18.28 (8.96)	A7a	15.71 (7.85)

TABLE S2: Coordination number of water around COS. The normalised values with respect to the density of water in the pure water system are given in the parenthesis.

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System	urea-water (vdW)	urea-water (elec)
S1	-1.04 (± 0.02)	-18.97 (± 0.13)
S7	-1.67 (± 0.03)	-23.47 (± 0.17)
A1	-0.97 (± 0.01)	-15.17 (± 0.11)
A7	-1.52 (± 0.03)	-19.47 (± 0.16)
System	COS-water (vdW)	COS-water (elec)
S4	-4.47 (± 0.07)	-60.32 (± 0.38)
S7	-8.75 (± 0.09)	-94.55 (± 0.61)
A4	-3.94 (± 0.04)	-46.65 (± 0.43)
A7	-8.72 (± 0.07)	-79.14 (± 0.52)
System	water-water (vdW)	water-water (elec)
S0	1.54 (± 0.03)	-7.35 (± 0.08)
S1	1.17 (± 0.01)	-7.90 (± 0.06)
S2	1.03 (± 0.02)	-7.96 (± 0.04)
S3	1.08 (± 0.03)	-8.39 (± 0.10)
S4	1.11 (± 0.03)	-8.98 (± 0.08)
S5	0.96 (± 0.02)	-9.65 (± 0.07)
S6	0.78 (± 0.01)	-10.38 (± 0.05)
S7	0.72 (± 0.01)	-10.68 (± 0.04)
S7a	0.74 (± 0.01)	-10.21 (± 0.07)
A0	1.41 (± 0.03)	-7.30 (± 0.04)
A1	1.27 (± 0.02)	-7.71 (± 0.06)
A2	1.11 (± 0.02)	-7.88 (± 0.08)
A3	1.19 (± 0.01)	-8.28 (± 0.05)
A4	1.23 (± 0.02)	-8.43 (± 0.05)
A5	1.01 (± 0.02)	-9.32 (± 0.07)
A6	0.93 (± 0.01)	-10.35 (± 0.08)
A7	0.87 (± 0.01)	-10.80 (± 0.04)
A7a	0.92 (± 0.01)	-10.72 (± 0.09)

TABLE S3: vdW and electrostatic interaction energies between urea and water (per urea molecules) for systems S1, A1 (8 M urea) and S7, A7 (1.0 M COS + 8 M urea); between COS and water for systems S4, A4 (1.0 M COS) and S7, A7 (1.0 M COS + 8 M urea); and between water-water for all the systems studied here (systems S0, A0 to S7a, A7a). Energies are expressed in kcal/mol unit. Errors are given in the parenthesis.