

Electronic supplementary information for

Thermodynamic characterization of the biocompatible ionic liquid effects on protein model compounds and their functional groups

Pankaj Attri and Pannuru Venkatesu*

Department of Chemistry, University of Delhi, Delhi – 110 007, India

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Table 1 Cyclic dipeptide solubilities (S_{cd}) in water or in aqueous ILs and densities (ρ^{*}_{cd}) at solubility limits at 25 °C

Co-solvents	S_{cd} (g/100 g of solvent)				ρ^{*}_{cd}			
	0 % (v/v)	30% (v/v)	50% (v/v)	70% (v/v)	0 % (v/v)	30% (v/v)	50% (v/v)	70% (v/v)
c(GG) (MW) = 114.10 g mol⁻¹								
water	1.68				1.00250			
DEAA		1.230	0.990	0.700		1.00342	1.01356	1.11230
TEAA		1.170	0.918	0.639		1.00305	1.01489	1.05353
DEAP		1.350	1.130	0.862		1.00516	1.01377	1.12755
TEAP		1.31	1.040	0.822		1.00423	1.10103	1.11046
DEAS		1.09	0.739	0.521		1.00187	1.06566	1.11523
TEAS		0.980	0.659	0.402		1.00069	1.02139	1.12344
c(AG) (MW) = 128.13 g mol⁻¹								
water	7.31				1.01549			
DEAA		4.710	3.250	2.160		1.00468	1.05979	1.16381
TEAA		4.300	2.710	1.680		1.01487	1.06168	1.14353
DEAP		5.230	3.900	2.690		1.00791	1.03510	1.13885
TEAP		4.990	3.600	2.500		1.00390	1.05102	1.11360
DEAS		3.900	2.284	1.420		1.00239	1.09181	1.12829
TEAS		3.430	1.980	1.090		1.00221	1.04472	1.12310
c(AA) (MW) = 142.16 g mol⁻¹								
water	2.55				1.00238			
DEAA		1.530	1.040	0.670		1.00259	1.01143	1.08069
TEAA		1.450	0.980	0.560		1.00230	1.01311	1.04356
DEAP		1.920	1.400	0.970		1.00075	1.01077	1.11209
TEAP		1.760	1.310	0.860		1.00139	1.00790	1.10961
DEAS		1.300	0.760	0.430		1.00011	1.06284	1.12598
TEAS		1.200	0.670	0.340		1.00011	1.01965	1.11732
c(LA) (MW) = 184.24 g mol⁻¹								
water	0.328				0.99750			

DEAA	0.190	0.130	0.084	1.00199	1.00271	1.06129
TEAA	0.166	0.106	0.060	1.00148	1.01263	1.03356
DEAP	0.231	0.182	0.142	1.00030	1.01031	1.09224
TEAP	0.214	0.156	0.106	1.00080	1.00224	1.10763
DEAS	0.140	0.076	0.036	0.99984	1.01948	1.10268
TEAS	0.122	0.057	0.018	0.99974	1.00703	1.10569
c(VV) (MW) = 198.27 g mol ⁻¹)						
water	0.0273			0.99711		
DEAA		0.0235	0.0210	0.0186	1.00047	1.01197
TEAA		0.0220	0.0190	0.0160	1.01071	1.01210
DEAP		0.0256	0.0240	0.0220	0.99950	1.00415
TEAP		0.0246	0.0222	0.0200	1.00055	1.02728
DEAS		0.0203	0.0165	0.0129	1.02496	1.04902
TEAS		0.0191	0.0140	0.0101	1.00569	1.07238

Table 2 Apparent transfer free energies $\Delta G'_{tr}$ of cds from water to aqueous ILs solution at 25 °C and at atmospheric pressure

CD	ILs	$\Delta G'_{tr}$ (J mol ⁻¹)		
		30% (v/v)	50% (v/v)	70% (v/v)
c(GG)	DEAA	759.60	1266.90	1888.57
	TEAA	883.03	1449.06	2076.48
	DEAP	527.49	941.92	1342.75
	TEAP	603.36	1037.03	1497.43
	DEAS	1059.56	1861.34	2609.77
	TEAS	1323.50	2248.56	3231.43
c(AG)	DEAA	1055.36	1807.94	2562.30
	TEAA	1246.38	2240.97	3217.20
	DEAP	800.07	1429.97	2084.90
	TEAP	920.75	1583.39	2317.49
	DEAS	1509.57	2585.25	3660.92
	TEAS	1817.12	3041.23	4312.46
c(AA)	DEAA	1241.01	2164.25	3080.96
	TEAA	1372.90	2440.60	3609.49
	DEAP	692.22	1335.25	2100.08
	TEAP	902.40	1607.38	2401.28
	DEAS	1645.35	2812.01	4072.62
	TEAS	1841.33	3225.09	4671.72
c(LA)	DEAA	1338.92	2276.41	3217.09
	TEAA	1674.34	2757.36	4112.13
	DEAP	859.74	1424.87	1845.81
	TEAP	1047.59	1826.25	2535.06
	DEAS	2100.05	3564.66	5221.50
	TEAS	2441.01	4316.51	6021.20
c(VV)	DEAA	363.12	613.55	905.75
	TEAA	501.32	861.27	1276.00
	DEAP	153.40	301.83	415.20
	TEAP	249.56	438.60	600.55

DEAS	655.92	1122.14	1589.75
TEAS	864.04	1474.78	2204.47
