

Electronic Supplementary information of

Dielectric spectroscopy in the GHz region on fully hydrated
zwitterionic aminoacids

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TABLE 1. Data corresponding to the amino acids used in this work. M_w is the
molecular weight and pI is the isoelectric point.

<i>Amino Acid (NOTATION)</i>	M_w [g/mol]	<i>Solubility (20°C) [g/dL]</i>	<i>pI</i>
L-Glycine (GLY)	75.07	22.52	6.0
β-Alanine (β-ALA)	89.09	--	6.9
L-Alanine (ALA)	89.09	15.0	6.0
L-Proline (PRO)	115.13	154.6	6.3
L-Threonine (THR)	119.12	10.6	5.6
L-Lysine (LYS)	146.19	Very soluble	9.7
L-Histidine (HIS)	155.15	4.19	7.6
L- Arginine (ARG)	174.20	14.8	10.8

TABLE 2. Parameters c and c_w are the analytical molar concentrations of the solute and of water, respectively. c_w^{app} is the apparent water concentration and Z_{ib} is the effective hydration number, i.e., the number of water molecules irrotationally bound to a solute molecule.

	c [mol/L]	$c_w(c)$ [mol/ L]	$c_w^{app}(c)$ [mol/ L]	Z_{ib}
GLY	0.44	54.31	52.01	5.21
	0.64	53.82	50.54	5.09
	0.87	53.26	48.79	5.13
	1.09	52.72	47.26	4.99
	1.26	52.31	46.95	4.25
	1.67	51.27	43.75	4.50
	2.34	49.53	41.27	3.53
ALA	0.39	54.07	51.28	7.14
	0.58	53.44	49.38	7.01
	0.79	52.70	47.12	7.05
	1.17	51.43	43.48	6.82
	1.53	50.19	40.15	6.58

TABLE 3. These set of tables shows the parameters obtained from the fitting procedure ($\Delta\epsilon_j$, τ_j , γ_j) for all the amino acids studied in this work. 1 corresponds to the amino acid relaxation whereas 2 correspond with the relaxation of water molecules.

L-Glycine

	Process 1			Process 2		
X	τ_1 [ps]	$\Delta\epsilon_1$	γ_1	τ_2 [ps]	$\Delta\epsilon_2$	γ_2
0.0041	31.98	9.06	1	8.41	71.50	1
0.0081	35.4	17.21	1	8.27	69.79	1
0.0118	37.5	23.70	1	8.19	67.94	1
0.0161	39.94	31.13	1	8.18	65.70	1
0.0203	42.21	38.19	1	8.18	63.75	1
0.0235	44.06	42.23	1	8.18	63.40	1
0.0315	47.47	55.78	1	8.22	59.22	1
0.0451	54.73	75.30	1	8.53	56.05	1

β -Alanine

	Process 1			Process 2		
X	τ_1 [ps]	$\Delta\epsilon_1$	γ_1	τ_2 [ps]	$\Delta\epsilon_2$	γ_2
0.00349	52.30	8.77	1	8.91	71.89	1
0.00693	56.04	16.86	1	9.05	69.82	1
0.01004	58.76	24.46	0.9913	9.13	67.80	1
0.01342	61.98	32.18	0.9885	9.26	66.09	1
0.01993	68.71	46.50	0.9849	9.57	63.26	1
0.02619	74.72	59.75	0.9814	9.83	60.64	1
0.03126	80.76	69.20	0.9842	10.23	59.95	1

L-Alanine

	Process 1			Process 2		
X	τ_1 [ps]	$\Delta\epsilon_1$	γ_1	τ_2 [ps]	$\Delta\epsilon_2$	γ_2
0.0036	49.59	7.64	1	8.37	71.60	1
0.0072	51.55	14.85	1	8.40	68.72	1
0.0107	54.49	21.60	1	8.54	66.28	1
0.0148	57.83	29.27	0.99	8.50	63.37	1
0.0222	63.32	42.60	0.98	8.56	58.64	1
0.0295	71.76	56.41	0.98	8.86	54.29	1

L-Proline

	Process 1			Process 2		
X	τ_1 [ps]	$\Delta\epsilon_1$	γ_1	τ_2 [ps]	$\Delta\epsilon_2$	γ_2
0.0026	45.61	4.74	1	8.33	70.84	1
0.0052	51.13	9.77	1	8.57	69.44	1
0.0080	52.93	14.32	1	8.79	66.74	1
0.0106	54.53	18.57	1	8.83	64.82	1
0.0208	64.75	34.47	1	9.55	58.68	1
0.0314	74.56	48.77	0.99	10.17	53.50	1
0.0497	100.20	68.93	0.99	11.87	50.68	0.95
0.0683	128.60	86.40	0.99	13.87	47.04	0.91
0.0958	181.30	106.60	0.98	18.06	44.48	0.83
0.1353	308.00	129.10	0.97	32.25	44.44	0.72

L-Threonine

	Process 1			Process 2		
X	$\tau_1[\text{ps}]$	$\Delta\epsilon_1$	γ_1	$\tau_2[\text{ps}]$	$\Delta\epsilon_2$	γ_2
0.0025	59.15	4.53	1	8.01	72.00	1
0.0050	69.77	8.24	1	8.10	70.68	1
0.0075	75.07	12.15	1	8.23	69.03	1
0.0100	79.34	16.04	0.99	8.19	67.59	1
0.0125	84.76	19.53	0.99	8.46	66.57	1
0.0149	89.16	23.44	0.98	8.54	65.17	1

L-Lysine

	Process 1			Process 2		
X	$\tau_1[\text{ps}]$	$\Delta\epsilon_1$	γ_1	$\tau_2[\text{ps}]$	$\Delta\epsilon_2$	γ_2
0.0044	147.2	19.66	0.94	8.49	69.90	1
0.0091	169.2	38.51	0.93	8.68	64.97	1
0.0138	202.7	56.51	0.92	9.15	61.55	1
0.0193	239.8	75.71	0.91	9.48	58.06	1
0.03008	336.3	107.20	0.91	10.63	55.16	1

L-Histidine

	Process 1			Process 2		
X	$\tau_1[\text{ps}]$	$\Delta\epsilon_1$	γ_1	$\tau_2[\text{ps}]$	$\Delta\epsilon_2$	γ_2
0.0020	83.16	5.68	1	9.05	71.92	1
0.0027	86.09	7.44	1	9.10	71.23	1
0.0035	92.88	9.25	1	9.17	70.40	1
0.0042	98.24	11.07	1	9.21	69.78	1
0.0046	99.52	11.89	1	9.20	69.35	1

L- Arginine

	Process 1			Process 2		
X	$\tau_1[\text{ps}]$	$\Delta\epsilon_1$	γ_1	$\tau_2[\text{ps}]$	$\Delta\epsilon_2$	γ_2
0.0021	173.2	10.66	0.93	8.93	71.66	1
0.0036	181.0	17.90	0.94	8.86	69.68	1
0.0053	196.1	26.00	0.93	9.03	67.80	1
0.0069	209.2	33.84	0.93	9.07	65.91	1
0.0092	229.1	44.36	0.92	9.17	63.51	1
0.0105	235.1	49.55	0.92	9.07	62.17	1