Supplementary Material: Theoretical investigation of glycine micro-solvated. Energy and NMR spin spin coupling constants calculations

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1 Energy

Energies for the different super-molecular systems of Gly:$(H_2O)_n$ (with n = 1 to 8) incorporating water molecules one-by-one according to Table 1 were obtained as: $E_{Gly} + (8 - n) \cdot E_{H_2O}$, where E_{Gly} and E_{H_2O} are the energies of glycine and water respectively within the PCM model.

Table S1 Energy [in a. u.] for the N-, TS- and Z-Glycine super-molecular systems with 0 to 8 water molecules.

N°of W	N-Gly	TS-Gly	Z-Gly
0W	−896.063	−896.059	−896.072
1W	−896.067	−896.064	−896.078
2W	−896.069	−896.067	−896.084
3W	−896.074	−896.073	−896.092
4W	−896.076	−896.075	−896.097
5W	−896.081	−896.080	−896.104
6W	−896.085	−896.084	−896.113
7W	−896.089	−896.089	−896.117
8W	−896.097	−896.094	−896.125

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2 SSCC's

Intra-molecular SSCC's between the heavy atoms, other than hydrogen, from one- to three-bonds in glycine neutral and it zwitterion have been investigated for the neutral and zwitterionic forms in a electrostatic embedding within PCM and adding to the calculations up to 8 molecules in explicit form.

Table S2 One- two- and three-bond spin-spin coupling constants (in Hz) obtained at the B3LYP/6-31G** level of calculations using PCM for both neutral (N) and zwitterionic (Z) conformers in function of the number of water molecules.

Coupling	Molecule	0W					1W					2W				
		FC	SD	PSO	DSO	Total	FC	SD	PSO	DSO	Total	FC	SD	PSO	DSO	Total
$^1J(C_{O's}, C_N)$	N	57.22	0.72	−1.87	0.32	56.38	57.29	0.72	−1.87	0.32	56.45	56.82	0.72	−1.88	0.33	55.99
	Z	55.25	0.86	−1.38	0.32	55.04	54.68	0.85	−1.44	0.32	54.42	58.29	0.68	−1.17	0.33	58.12
$^1J(N, C_N)$	N	−4.21	−0.79	−0.16	−0.08	−5.24	−4.27	−0.79	−0.16	−0.08	−5.31	−4.33	−0.78	−0.13	−0.09	−5.32
	Z	−2.65	−0.94	−0.42	−0.08	−4.09	−2.92	−0.96	−0.51	−0.08	−4.48	−6.36	−0.77	−0.41	−0.09	−7.64
$^1J(O_{Ac}, C_{O's})$	N	20.77	−0.01	8.77	−0.14	29.38	19.94	−0.00	8.56	−0.15	28.34	19.59	−0.01	8.64	−0.15	28.06
	Z	23.87	−0.40	11.76	−0.13	35.11	23.96	−0.29	11.36	−0.14	34.89	22.71	−0.22	9.35	−0.15	31.68
$^1J(O_T, C_{O's})$	N	16.74	−1.63	13.54	−0.11	28.53	16.76	−1.69	13.56	−0.12	28.51	16.89	−1.64	13.56	−0.12	28.70
	Z	22.54	−0.41	11.69	−0.13	33.69	21.82	−0.56	11.97	−0.13	33.10	23.28	−0.40	9.83	−0.14	32.56
$^2J(N, C_{O's})$	N	−5.07	−0.02	0.16	−0.02	−4.94	−4.95	−0.02	0.16	−0.02	−4.83	−4.57	−0.02	0.17	−0.02	−4.45
	Z	0.01	0.01	0.07	−0.02	0.06	−0.04	0.00	0.06	−0.02	−0.00	−0.01	0.00	0.05	−0.02	0.02
$^2J(O_{Ac}, C_N)$	N	−2.57	0.03	0.68	0.01	−1.85	−3.01	0.04	0.67	0.01	−2.30	−2.93	0.04	0.68	0.01	−2.21
	Z	−7.56	−0.19	0.79	0.02	−6.94	−7.73	−0.14	0.77	0.01	−7.08	−5.18	−0.11	0.66	0.01	−4.62
$^2J(O_T, C_N)$	N	−4.60	−0.13	1.38	0.03	−3.32	−4.47	−0.13	1.40	0.03	−3.18	−4.38	−0.14	1.40	0.03	−3.10
	Z	−11.63	0.00	0.79	0.01	−10.83	−10.53	−0.02	0.92	0.01	−9.62	−6.26	−0.02	0.78	0.01	−5.49
$^2J(O_T, O_{Ac})$	N	4.81	1.00	−6.29	−0.03	−0.51	4.45	0.97	−6.26	−0.03	−0.87	4.29	0.98	−6.25	−0.03	−1.01
	Z	1.38	1.44	−7.29	−0.04	−4.50	0.90	1.38	−7.10	−0.04	−4.86	0.01	1.11	−5.74	−0.03	−4.65
$^3J(O_{Ac}, N)$	N	2.60	−0.04	−0.33	0.00	2.23	3.18	−0.04	−0.34	0.01	2.81	3.70	−0.04	−0.37	0.01	3.30
	Z	0.75	−0.01	−0.14	0.00	0.61	1.71	−0.01	−0.18	0.01	1.53	0.77	−0.01	−0.15	0.01	0.62
$^3J(O_T, N)$	N	0.41	0.00	−0.01	−0.02	0.37	0.40	0.00	−0.01	−0.02	0.37	0.36	0.00	−0.01	−0.02	0.34
	Z	0.25	−0.02	0.01	−0.02	0.22	0.24	−0.02	0.05	−0.02	0.24	0.32	−0.02	0.03	−0.02	0.31

Table S3 One- two- and three-bond spin-spin coupling constants (in Hz) obtained at the B3LYP/6-31G** level of calculations using PCM for both neutral (N) and zwitterionic (Z) conformers in function of the number of water molecules.

Coupling	Molecule	3W					4W					5W				
		FC	SD	PSO	DSO	Total	FC	SD	PSO	DSO	Total	FC	SD	PSO	DSO	Total
$^1J(C_{O's}, C_N)$	N	56.72	0.72	−1.93	0.33	55.84	56.31	0.73	−1.93	0.33	55.44	54.99	0.73	−1.99	0.34	54.07
	Z	55.65	0.85	−1.49	0.33	55.33	55.85	0.84	−1.51	0.34	55.51	57.28	0.84	−1.55	0.35	56.91
$^1J(N, C_N)$	N	−4.55	−0.77	−0.11	−0.09	−5.52	−4.66	−0.76	−0.08	−0.09	−5.59	−4.88	−0.76	−0.06	−0.09	−5.79
	Z	−3.55	−0.95	−0.48	−0.09	−5.07	−3.82	−0.95	−0.45	−0.09	−5.31	−3.83	−0.93	−0.38	−0.10	−5.24
$^1J(O_{Ac}, C_{O's})$	N	19.37	−0.02	8.85	−0.16	28.03	19.05	−0.03	8.92	−0.16	27.79	17.78	−0.06	9.23	−0.16	26.80
	Z	23.63	−0.36	11.58	−0.15	34.70	23.59	−0.37	11.62	−0.15	34.69	22.78	−0.47	12.02	−0.15	34.18
$^1J(O_T, C_{O's})$	N	16.93	−1.54	13.49	−0.13	28.75	17.09	−1.49	13.49	−0.13	28.97	16.40	−1.32	13.46	−0.14	28.41
	Z	22.03	−0.45	11.80	−0.14	33.24	22.22	−0.43	11.81	−0.14	33.46	21.86	−0.29	11.57	−0.15	32.99
$^2J(N, C_{O's})$	N	−4.57	−0.02	0.17	−0.02	−4.44	−4.21	−0.02	0.18	−0.03	−4.08	−3.97	−0.02	0.18	−0.03	−3.83
	Z	0.03	0.00	0.07	−0.02	0.07	0.11	0.00	0.07	−0.03	0.16	0.06	0.00	0.09	−0.03	0.13
$^2J(O_{Ac}, C_N)$	N	−2.59	0.04	0.70	0.01	−1.85	−2.54	0.04	0.71	0.00	−1.79	−2.09	0.04	0.74	0.00	−1.31
	Z	−7.42	−0.14	0.83	0.01	−6.72	−7.47	−0.14	0.84	0.01	−6.76	−7.38	−0.16	0.89	0.00	−6.65
$^2J(O_T, C_N)$	N	−4.94	−0.12	1.37	0.02	−3.67	−4.88	−0.13	1.36	0.02	−3.63	−4.07	−0.12	1.35	0.01	−2.82
	Z	−11.51	−0.01	0.91	0.00	−10.60	−11.41	−0.01	0.92	0.00	−10.49	−10.45	0.00	0.86	−0.00	−9.59
$^2J(O_T, O_{Ac})$	N	3.59	0.98	−6.19	−0.02	−1.65	3.45	0.99	−6.17	−0.02	−1.75	3.92	1.03	−5.95	−0.02	−1.02
	Z	0.55	1.33	−7.12	−0.03	−5.27	0.55	1.31	−7.12	−0.03	−5.29	0.85	1.30	−7.23	−0.03	−5.10
$^3J(O_{Ac}, N)$	N	3.97	−0.04	−0.37	0.01	3.57	4.49	−0.04	−0.40	0.01	4.06	5.14	−0.04	−0.43	0.01	4.68
	Z	1.52	−0.01	−0.17	0.01	1.34	1.34	−0.01	−0.17	0.01	1.17	0.46	−0.00	−0.12	0.01	0.35
$^3J(O_T, N)$	N	0.40	−0.00	−0.01	−0.02	0.37	0.35	0.00	−0.00	−0.02	0.33	0.24	0.00	0.00	−0.02	0.23
	Z	0.25	−0.02	0.04	−0.02	0.25	0.23	−0.02	0.03	−0.02	0.22	0.19	−0.01	−0.03	−0.02	0.13

Table S4 One- two- and three-bond spin-spin coupling constants (in Hz) obtained at the B3LYP/6-31G** level of calculations using PCM for both neutral (N) and zwitterionic (Z) conformers in function of the number of water molecules.

Coupling	Molecule	6W					7W					8W				
		FC	SD	PSO	DSO	Total	FC	SD	PSO	DSO	Total	FC	SD	PSO	DSO	Total
$^1J(C_{O's}, C_N)$	N	54.99	0.73	−2.01	0.35	54.06	54.72	0.72	−2.09	0.36	53.70	56.69	0.67	−2.11	0.36	55.61
	Z	57.49	0.82	−1.60	0.35	57.06	57.64	0.81	−1.68	0.36	57.13	58.38	0.79	−1.66	0.36	57.87
$^1J(N, C_N)$	N	−5.08	−0.75	−0.04	−0.10	−5.97	−5.07	−0.75	−0.03	−0.10	−5.95	−3.90	−0.77	−0.06	−0.10	−4.82
	Z	−3.92	−0.93	−0.39	−0.10	−5.33	−4.00	−0.93	−0.38	−0.10	−5.40	−3.97	−0.92	−0.41	−0.10	−5.40
$^1J(O_{Ac}, C_{O's})$	N	18.21	−0.05	9.04	−0.17	27.03	17.68	−0.09	9.33	−0.17	26.76	20.11	−0.02	8.61	−0.18	28.52
	Z	23.06	−0.30	11.66	−0.16	34.26	22.50	−0.43	12.00	−0.16	33.90	23.45	−0.18	11.41	−0.17	34.51
$^1J(O_T, C_{O's})$	N	16.19	−1.40	13.55	−0.14	28.19	16.25	−1.23	13.43	−0.15	28.29	15.28	−1.66	13.62	−0.14	27.10
	Z	21.33	−0.45	11.98	−0.16	32.70	21.66	−0.31	11.68	−0.17	32.86	20.88	−0.57	12.29	−0.16	32.43
$^2J(N, C_{O's})$	N	−3.83	−0.01	0.18	−0.03	−3.70	−3.80	−0.01	0.19	−0.03	−3.65	−3.83	−0.00	0.16	−0.03	−3.71
	Z	0.07	0.00	0.09	−0.03	0.13	0.08	0.00	0.10	−0.03	0.15	−0.10	−0.00	0.09	−0.03	−0.05
$^2J(O_{Ac}, C_n)$	N	−2.21	0.04	0.73	0.00	−1.44	−2.01	0.04	0.76	−0.00	−1.21	−2.42	0.02	0.73	−0.01	−1.68
	Z	−7.38	−0.16	0.89	−0.00	−6.65	−7.07	−0.16	0.94	−0.00	−6.29	−7.44	−0.16	0.91	−0.01	−6.69
$^2J(O_T, C_N)$	N	−4.01	−0.12	1.37	0.01	−2.76	−3.85	−0.12	1.37	0.01	−2.59	−3.99	−0.11	1.38	0.01	−2.71
	Z	−10.15	−0.00	0.90	−0.01	−9.25	−9.88	0.01	0.89	−0.01	−8.99	−10.15	0.00	0.94	−0.01	−9.22
$^2J(O_T, O_{Ac})$	N	3.85	0.98	−5.93	−0.02	−1.11	4.02	0.94	−5.83	−0.02	−0.88	4.90	0.91	−5.97	−0.01	−0.17
	Z	0.93	1.19	−7.12	−0.02	−5.02	1.00	1.08	−7.00	−0.02	−4.94	0.99	1.08	−7.03	−0.02	−4.99
$^3J(O_{Ac}, N)$	N	5.20	−0.05	−0.44	0.01	4.73	5.34	−0.05	−0.44	0.01	4.87	1.80	−0.03	−0.29	0.01	1.49
	Z	0.45	−0.00	−0.12	0.01	0.34	0.48	−0.01	−0.12	0.01	0.36	0.13	−0.00	−0.09	0.01	0.05
$^3J(O_T, N)$	N	0.24	−0.00	0.00	−0.02	0.22	0.22	−0.00	0.00	−0.02	0.20	0.31	−0.01	−0.03	−0.02	0.25
	Z	0.19	−0.01	−0.03	−0.02	0.14	0.17	−0.01	−0.03	−0.01	0.12	0.26	−0.00	−0.05	−0.01	0.20