Water-induced Zwitterionization of Glycine: Stabilization Mechanism and Spectral Signatures

Ricardo Pérez de Tudela* and Dominik Marx*

Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, 44780 Bochum, Germany

E-mail: ricardo.perez@theochem.rub.de; dominik.marx@theochem.rub.de

*To whom correspondence should be addressed

In this Supporting Information the structures, total energies and harmonic IR spectra (in terms of frequencies and intensities including O and N isotopic substitution) of all optimized species are compiled as obtained from (RI–) SCS–MP2/TZVPP structure optimizations and subsequent harmonic analysis (see main text for references).

- The optimized configurations corresponding to the global minimum structures for non–dissociated (N) and zwitterionic (Z) Gly•$(H_2O)_n$ clusters are shown in Table 1 together with their total dipole moments; the corresponding Cartesian coordinates and total energies can be found in Tables 5 to 23.

- In Table 2 the energy differences of the re–optimized $n = 9$ and 10 structures after one or two water molecules have been removed from the water bridge and placed somewhere else in a H–bonding configuration (first test set, see text) with respect to the respective global N minimum structure are compiled along with the corresponding Cartesian coordinates and total energies in Tables 24 to 74.

- Table 3 collects the energy differences resulting from the re–optimiziations for the second test set (see text), which consists of adding a water molecule to any of the free NH sites of glycine. The corresponding Cartesian coordinates and total energies can be found in Tables 75 to 83.

- In the third test set, the outermost water molecule bound to the $–NH_3^+$ group is artificially removed and the water molecule is and placed somewhere else in a H–bonding configuration. The energy differences of the optimized structures with respect to the respective global N minimum structure are tabulated in Table 4, and the Cartesian coordinates together with the total energies are collected in Tables 84 to 108.

- Finally, the harmonic IR spectra of the global non–dissociated and zwitterionic minima compiled in Table 1 are provided in terms of unscaled frequencies and IR intensities in Tables 109 to 127. Note that in each of these tables, the properties corresponding to the

natural majority isotope as well as to the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included; the masses used for the various isotopes can be found in Table 128.

In order to explore the configuration space, ab initio molecular dynamics (AIMD) simulations for zwitterionic and non-dissociated Gly$\bullet(H_2O)_n$ clusters (with $n = 1, \ldots, 10$) at 300 K were performed using the `CP2k` simulation package.[1] As initial configurations for these AIMD simulations the global minima from previous works[2,3] were taken. The density functional BLYP was chosen along with the 6-31G* basis set. For each of these cases, 20 time-equidistant structures were sampled along 10 ps AIMD trajectories and subsequently optimized using the SCS–(RI)–MP2/SVP method as implemented in the `Turbomole` package.[4] All the relevant configurations reported in the literature were recovered by this sampling procedure whereas no new, yet unknown structures were found. This provides some confidence that the set of structures which we use to investigate the H-bonding pattern in zwitterionic versus non-dissociated clusters is a reasonably exhaustive sample of representative structures.

Table 1: Global non–dissociated and zwitterionic optimized structures along with their dipole moments. The corresponding Cartesian coordinates and total energies can be found in Tables 5 to 23.

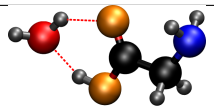
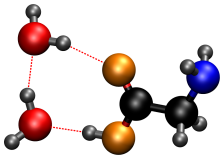
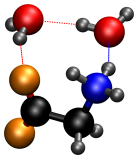
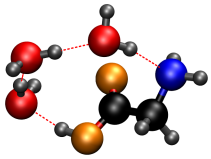
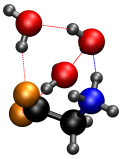
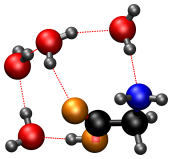
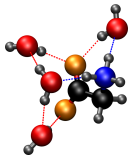
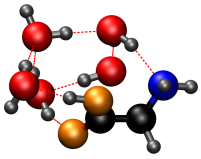
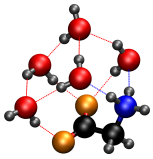
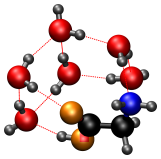
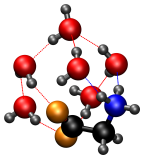
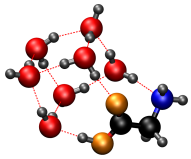
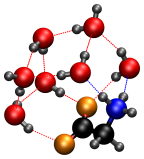
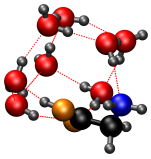
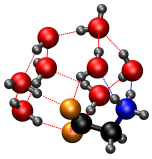
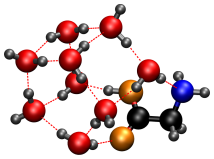
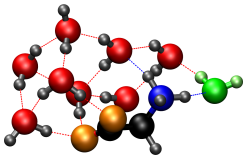
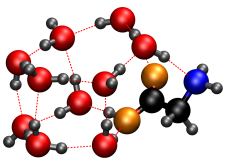
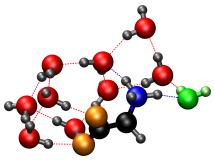
n	Non–dissociated	μ (D)	Zwitterionic	μ (D)
1		1.8		
2		1.4		6.8
3		4.0		4.4
4		4.2		3.7
5		2.1		4.8
6		1.9		2.8
7		2.7		4.5
8		4.6		3.6
9		1.9		3.1
10		1.9		4.5

Table 2: Relative energies (in kcal/mol) of the optimized structures from test set 1 with respect to the global non–dissociated minimum (N). The corresponding Cartesian coordinates and total energies can be found in Tables 24 to 74.

$n = 9$		$n = 10$	
Conformer	dZN	Conformer	dZN
gw9-bb-1	-3.5	gw10-bb-1	4.3
gw9-bb-2	6.8	gw10-bb-2	5.3
gw9-bb-3	1.3	gw10-bb-3	3.9
gw9-bb-4	2.7	gw10-bb-4	0.9
gw9-bb-5	2.7	gw10-bb-5	6.0
gw9-bb-6	-3.5	gw10-bb-6	-0.4
gw9-bb-7	7.2	gw10-bb-7	1.5
gw9-bb-8	4.2	gw10-bb-8	-2.7
gw9-bb-9	3.9	gw10-bb-9	1.8
gw9-bb-10	4.5	gw10-bb-10	4.3
gw9-bb-11	4.7	gw10-bb-11	2.2
gw9-bb-12	5.2	gw10-bb-12	1.4
gw9-bb-13	-1.3	gw10-bb-13	2.5
gw9-bb-14	6.5	gw10-bb-14	5.3
gw9-bb-15	-3.0	gw10-bb-15	1.0
gw9-bb-16	1.0	gw10-bb-17	5.8
gw9-bb-17	5.9	gw10-bb-18	5.5
gw9-bb-18	5.9	gw10-bb-19	3.8
gw9-bb-20	7.1	gw10-bb-21	7.4
gw9-bb-21	1.1	gw10-bb-22	4.9
		gw10-bb-23	4.0
		gw10-bb-24	3.5
		gw10-bb-25	-1.5
		gw10-bb-26	-3.6
		gw10-bb-27	0.6
		gw10-bb-28	1.1
		gw10-bb-29	1.1
		gw10-bb-30	2.9
		gw10-bb-31	3.4
		gw10-bb-32	1.8
		gw10-bb-33	2.9

Table 3: Relative energies (in kcal/mol) of the optimized structures from test set 2 with respect to the global non–dissociated minimum (N). The corresponding Cartesian coordinates and total energies can be found in Tables 75 to 83.

n	Structure	dZN
3	2Za-1	7.17
	2Za-2	12.42
4	3Za-1	8.71
	3Za-2	2.91
5	4Za-1	2.52
6	5Za-1	5.61
7	6Za-1	5.11
8	7Zb-1	4.38
9	8Za-1	0.73

Table 4: Relative energies (in kcal/mol) of the optimized structures from test set 3 with respect to the global non–dissociated minimum (N). The corresponding Cartesian coordinates and total energies can be found in Tables 84 to 108.

n	Structure	dZN
	gw9-rb	-3.5
	gw9-rb-1	3.2
	gw9-rb-2	-3.5
	gw9-rb-3	-3.5
	gw9-rb-4	3.0
9	gw9-rb-5	4.0
	gw9-rb-6	6.2
	gw9-rb-7	6.3
	gw9-rb-8	3.3
	gw9-rb-9	-3.4
	gw9-rb-10	-1.5
	gw9-rb-11	-1.3
	gw10-rb	-3.7
	gw10-rb-1	-3.7
	gw10-rb-2	-3.6
	gw10-rb-3	1.8
	gw10-rb-4	1.2
	gw10-rb-5	1.3
10	gw10-rb-6	1.3
	gw10-rb-8	-1.4
	gw10-rb-9	1.1
	gw10-rb-10	-1.9
	gw10-rb-11	2.8
	gw10-rb-12	-3.6
	gw10-rb-13	-1.2
	gw10-rb-14	-3.6

Table 5: Cartesian coordinates (in Angstrom) of the global non–dissociated Gly•$(H_2O)_1$ cluster.

13			
Energy = -360.3068640961			
C	0.1424418	0.0682343	0.0964725
O	1.4642354	-0.0376188	-0.0445906
H	1.6408553	-0.3831950	-0.9511884
O	-0.6659871	-0.2255389	-0.7684988
C	-0.2389628	0.5983520	1.4620454
H	0.1953045	-0.0724655	2.2030257
H	0.2693281	1.5533175	1.5923808
N	-1.6559279	0.7535928	1.7028756
H	-2.0486078	1.3732483	1.0061219
H	-2.1200346	-0.1338155	1.5589153
O	1.2833918	-0.8931410	-2.6029278
H	0.3576856	-0.8127299	-2.3197722
H	1.3762777	-1.7882403	-2.9348596

Table 6: Cartesian coordinates (in Angstrom) of the global non–dissociated Gly•$(H_2O)_2$ cluster.

16			
Energy = -436.6490150670			
C	-0.0230341	0.5978504	0.4442152
O	0.9292475	0.0104284	1.1477485
H	1.1882486	-0.8656080	0.7437601
O	-0.5332058	0.1434542	-0.5694475
C	-0.4270126	1.9305184	1.0422978
H	-0.7299423	1.7437721	2.0722115
H	0.4721350	2.5429264	1.1041157
N	-1.4685161	2.6488142	0.3423489
H	-1.1805639	2.8077784	-0.6143882
H	-2.2918356	2.0644566	0.2765177
O	1.7032633	-2.3092608	0.1323030
H	1.5931797	-3.0845290	0.6858206
H	1.1423656	-2.4664801	-0.6557976
O	-0.1049684	-2.2602380	-1.8568126
H	-0.3542755	-1.3838877	-1.5090630
H	0.0849148	-2.1199954	-2.7858302

Table 7: Cartesian coordinates (in Angstrom) of the global zwitterionic Gly•$(H_2O)_2$ cluster.

16			
Energy = -436.6319030555			
C	-0.2321435	1.3321918	0.8502311
H	-0.1926237	2.0458726	1.6670009
C	1.2028107	0.8723651	0.4684479
N	-0.9050494	0.0834127	1.2911592
H	-0.7367283	1.7666748	-0.0044515
O	1.4311961	-0.3337326	0.8621179
O	1.9166502	1.6437990	-0.1562956
H	-1.4156384	-0.3401775	0.5013668
H	0.0203166	-0.4985192	1.3974409
H	-1.4738833	0.1653727	2.1224706
O	1.1809566	-1.3791417	-1.6517426
H	1.4877802	-1.1434842	-0.7525362
H	1.6719880	-0.7775734	-2.2173257
O	-1.4417953	-0.8709414	-1.2077390
H	-1.9957816	-1.4854701	-1.6909802
H	-0.5180547	-1.0806486	-1.4791645

Table 8: Cartesian coordinates (in Angstrom) of the global non–dissociated Gly•$(H_2O)_3$ cluster.

19			
Energy = -512.9884022503			
C	0.5728837	0.6488420	0.8426780
O	1.8003409	0.2118045	0.6106367
H	2.1186584	0.6592108	-0.2299189
O	0.0294111	1.5682502	0.2585158
C	-0.1161223	-0.1176236	1.9487907
H	0.1663831	-1.1652109	1.8816861
H	0.2632066	0.2704986	2.8984441
N	-1.5594365	0.0291391	1.7751345
H	-2.0523356	-0.2489465	2.6126722
H	-1.7570472	1.0082031	1.6008004
O	-1.6368710	-1.3224376	-0.6821183
H	-2.4891502	-1.2545257	-1.1166246
H	-1.7538936	-0.8517426	0.1747961
O	0.3909718	-0.7107121	-2.4714715
H	0.7452413	-1.5820977	-2.6570167
H	-0.3143460	-0.8717754	-1.8139798
O	2.2491407	1.1860903	-1.7777618
H	1.7430292	2.0023381	-1.7256201
H	1.5999356	0.5406954	-2.1296428

Table 9: Cartesian coordinates (in Angstrom) of the global zwitterionic Gly•$(H_2O)_3$ cluster.

19			
Energy = -512.9798325560			
C	-0.4605311	-0.9080908	1.3198127
H	-0.5977539	-1.2175157	2.3524206
C	-0.2156865	0.6208980	1.2564648
N	0.7894132	-1.5057907	0.7814063
H	-1.3050511	-1.2136034	0.7129495
O	0.9990613	0.9304296	1.4169534
O	-1.1988664	1.3476625	1.0374593
H	0.9421912	-2.4776660	1.0207738
H	0.7616623	-1.3334455	-0.2704384
H	1.5172789	-0.8747620	1.1570945
O	-2.1546837	0.1427347	-1.1766634
H	-1.9815701	0.6851930	-0.3745677
H	-2.7778154	0.6468687	-1.7020841
O	0.4591494	-0.6331508	-1.6844331
H	-0.4819983	-0.3701652	-1.6978736
H	0.9392641	0.2207027	-1.6393561
O	1.7639880	1.7076468	-1.0620857
H	1.5401705	1.6571794	-0.1098025
H	1.4617777	2.5748747	-1.3380303

Table 10: Cartesian coordinates (in Angstrom) of the global non–dissociated Gly•$(H_2O)_4$ cluster.

22

Energy = -589.3309110326

C	-0.6677284	1.0467190	0.4892904
O	-0.1143483	1.0397409	1.6812089
H	0.8714234	1.2541369	1.6058740
O	-0.1047095	1.3361363	-0.5559856
C	-2.1328442	0.6781627	0.5349796
H	-2.2578328	-0.1568675	1.2204345
H	-2.6605061	1.5365457	0.9599425
N	-2.5790963	0.3088100	-0.8058430
H	-3.5838936	0.3893841	-0.8816891
H	-2.1626641	0.9564744	-1.4658779
O	-1.1956826	-2.1275471	-0.9606551
H	-1.7821185	-1.3410000	-1.0287425
H	-1.5846452	-2.7850910	-1.5397978
O	3.2479350	-0.8634800	0.4404004
H	3.3297296	-1.6721963	0.9475712
H	2.5671266	-1.0480120	-0.2458431
O	1.3282820	-1.0185669	-1.4427677
H	0.5107640	-1.5308015	-1.3062134
H	1.0106572	-0.1083299	-1.3905902
O	2.4416228	1.4233710	1.5784079
H	2.7183465	2.1005862	0.9571151
H	2.8001825	0.5818250	1.2087809

Table 11: Cartesian coordinates (in Angstrom) of the global zwitterionic Gly•$(H_2O)_4$ cluster.

22			
Energy = -589.3262806943			
C	-0.5311918	-0.4722136	1.4037256
H	-0.2898201	-0.4568516	2.4640024
C	-0.3413639	0.9339023	0.7994824
N	0.3943878	-1.4191518	0.7176444
H	-1.5482191	-0.8175684	1.2536189
O	0.8621287	1.3131806	0.6807685
O	-1.3665756	1.5510916	0.4633278
H	0.2130415	-2.3784465	0.9936111
H	0.2381660	-1.3108493	-0.3309781
H	1.3761634	-1.1800655	0.9570223
O	-2.7509882	-0.2463365	-0.9518934
H	-3.5489316	0.0623823	-1.3837815
H	-2.4248269	0.5115072	-0.4152914
O	-0.2092152	-0.9061554	-1.8143132
H	0.2080564	-0.0463829	-2.0357733
H	-1.1603375	-0.7019216	-1.7360451
O	0.9848578	1.5686001	-2.0219398
H	0.4571671	2.2982901	-2.3529063
H	0.9910028	1.6985298	-1.0511641
O	2.6948621	-0.3016743	1.6715913
H	2.1710200	0.4774593	1.3632448
H	3.5806164	-0.1773257	1.3260468

Table 12: Cartesian coordinates (in Angstrom) of the global non–dissociated Gly•$(H_2O)_5$ cluster.

25
Energy = -665.6736670025

C	0.9080837	0.2487278	1.2658438
O	2.0363585	0.4326314	0.5981978
H	2.3858862	-0.4692576	0.3268661
O	0.5126834	-0.8356255	1.6612422
C	0.1663604	1.5367575	1.5302974
H	-0.8953707	1.3016927	1.5277837
H	0.4378926	1.8501393	2.5436061
N	0.4480402	2.5340845	0.4986798
H	-0.0213312	3.4022886	0.7203308
H	1.4416655	2.7224247	0.4651290
O	0.3327132	-1.5288533	-1.8518305
H	0.3054276	-1.7527699	-2.7846214
H	0.0607689	-0.5712342	-1.8046918
O	2.6137996	-1.9305104	-0.3565927
H	2.3310484	-2.5450211	0.3266239
H	1.8484903	-1.8854365	-0.9658341
O	-1.6121479	-2.0545997	0.2193808
H	-0.9993386	-1.8017403	0.9241089
H	-1.0346047	-2.0872979	-0.5583579
O	-0.5736858	0.9345103	-1.6276214
H	-1.4601019	0.8324538	-1.2365901
H	-0.1412148	1.5882759	-1.0410112
O	-2.8165318	0.3532828	-0.1120112
H	-2.5211356	-0.5718228	0.0350774
H	-3.7537557	0.2969001	-0.3040054

Table 13: Cartesian coordinates (in Angstrom) of the global zwitterionic Gly•$(H_2O)_5$ cluster.

25			
Energy = -665.6724992618			
C	-0.9998365	2.1328665	-0.3708778
H	-0.3854018	3.0201366	-0.4754506
C	-0.5137293	1.0276148	-1.3284664
N	-0.8594450	1.6113484	1.0193685
H	-2.0468179	2.3671503	-0.5444365
O	-1.1667415	-0.0510954	-1.2783263
O	0.4960332	1.2951719	-2.0111755
H	-1.5142660	0.7967230	1.1692400
H	0.1094195	1.2202661	1.1571316
H	-1.0455178	2.3280105	1.7125367
O	-2.3670474	-0.6236996	1.0920611
H	-2.1950882	-0.5857158	0.1295561
H	-1.7205053	-1.2865054	1.3866423
O	2.4837456	-0.2776578	-1.2886244
H	3.3181968	-0.0915172	-1.7230907
H	1.8146587	0.3006725	-1.7301029
O	1.4806423	0.2870180	1.2842888
H	1.1307603	-0.6009601	1.4784296
H	1.9844119	0.1637833	0.4591522
O	0.0400349	-2.1191990	1.4386105
H	0.1946945	-2.2870038	0.4677301
H	0.2303809	-2.9492305	1.8804837
O	0.4259824	-2.2633343	-1.1620853
H	1.2924921	-1.8704502	-1.3391487
H	-0.1870565	-1.5443928	-1.4234461

Table 14: Cartesian coordinates (in Angstrom) of the global non–dissociated Gly•$(H_2O)_6$ cluster.

28
Energy = -742.0182745729

C	-1.1172466	-1.0945119	0.7056413
O	-2.0290112	-0.1816837	0.4152725
H	-2.1628147	-0.1356101	-0.5657042
O	-0.6288552	-1.8815076	-0.0878768
C	-0.7478647	-1.0843882	2.1666609
H	-0.6486629	-0.0470269	2.4798378
H	-1.5917009	-1.5201251	2.7106701
N	0.5156911	-1.7930281	2.3409789
H	0.6734286	-2.0039524	3.3168251
H	0.4750088	-2.6684399	1.8330590
O	0.0299173	-1.1686347	-2.7382350
H	-0.1383069	-1.6917174	-1.9403053
H	0.8127081	-0.6466194	-2.4864803
O	-2.0396221	0.3540217	-2.1998169
H	-1.2983345	-0.2082349	-2.5538262
H	-2.7407907	0.3299539	-2.8535542
O	1.9792460	0.4917665	-1.6196139
H	2.0779284	0.2865877	-0.6512223
H	2.8672818	0.6690803	-1.9354796
O	0.2752342	2.1700478	1.5486325
H	0.0027338	2.2810670	0.6119978
H	0.4485192	3.0595405	1.8613469
O	2.1119630	0.1688675	0.9964605
H	1.5855428	0.9280214	1.3067284
H	1.7133238	-0.5965883	1.4574089
O	-0.1475557	2.3146404	-1.1380677
H	0.6226052	1.8077625	-1.4421808
H	-0.9003660	1.8607111	-1.5391574

Table 15: Cartesian coordinates (in Angstrom) of the global zwitterionic Gly•$(H_2O)_6$ cluster.

28
Energy = -742.0164847101

C	1.9904510	0.0132432	1.2783277
H	2.1636605	1.0194075	1.6457371
C	0.5178992	-0.3919834	1.4710599
N	2.3239687	-0.0271305	-0.1698246
H	2.6293316	-0.6909154	1.8057296
O	-0.2025102	0.4200395	2.1022330
O	0.1885080	-1.4964094	0.9736065
H	3.3018930	0.1865903	-0.3343912
H	2.0999323	-0.9592134	-0.5976731
H	1.7133603	0.6765878	-0.6899734
O	-0.6695343	-0.6800622	-2.4490018
H	-1.3324169	-0.8875072	-1.7347787
H	-1.1448424	-0.7685859	-3.2777550
O	1.4211015	-2.3253131	-1.3489815
H	0.9237621	-2.4265010	-0.5196210
H	0.7576068	-1.9273194	-1.9370091
O	-2.1804907	-1.2991381	-0.3896395
H	-1.4451871	-1.5114328	0.2187447
H	-2.6488873	-0.6012809	0.0952318
O	0.6375867	1.5701585	-1.4364610
H	0.0713085	0.9204399	-1.8910349
H	0.0529581	2.0460073	-0.8066143
O	-2.8148757	0.7314279	1.4633583
H	-3.4522290	0.6349160	2.1734278
H	-1.9457925	0.4959278	1.8566314
O	-0.7817666	2.6951611	0.5997937
H	-0.4480780	2.0789436	1.2743922
H	-1.7267175	2.5039425	0.6244855

Table 16: Cartesian coordinates (in Angstrom) of the global non–dissociated Gly•$(H_2O)_7$ cluster.

31
Energy = -818.3617002273

C	0.8108921	0.6210916	2.0243784
O	1.7837788	-0.2620703	2.0211470
H	2.1799905	-0.3366498	1.0962813
O	0.5844464	1.4371690	1.1455455
C	-0.0438813	0.5542189	3.2691179
H	-0.0656502	-0.4711384	3.6273797
H	0.4444584	1.1665659	4.0338129
N	-1.3929546	0.9900609	2.9176208
H	-1.9603674	1.0954017	3.7478600
H	-1.3304813	1.8960578	2.4679270
O	1.8097873	0.2406500	-2.8024094
H	1.0382768	-0.3636423	-2.9473265
H	2.3207523	0.2218645	-3.6136600
O	-1.8886981	-0.8231059	0.7197230
H	-1.8340861	-0.2151805	1.4835976
H	-2.0638502	-0.2500035	-0.0451994
O	-2.0245469	0.6552478	-1.6979037
H	-1.2605794	1.2875381	-1.6518799
H	-2.7637964	1.1582056	-2.0445488
O	-0.3559519	-1.3019861	-2.8752391
H	-0.2692784	-1.8573824	-2.0832813
H	-1.0793355	-0.6974662	-2.6420977
O	0.1659552	2.1342150	-1.5292505
H	0.4490825	1.9882981	-0.6138759
H	0.8317167	1.6659997	-2.0578159
O	2.4908144	-0.9845003	-0.3347936
H	2.4313133	-0.4839807	-1.1649059
H	1.7230802	-1.5810078	-0.3645785
O	0.0274003	-2.3767902	-0.2884294
H	-0.6523623	-1.8322301	0.1835553
H	-0.1059254	-3.2754499	0.0192492

Table 17: Cartesian coordinates (in Angstrom) of the global zwitterionic Gly•$(H_2O)_7$ cluster.

31
Energy = -818.3614430286

C	0.1512299	-0.9147796	2.6161377
H	0.3921857	-1.9687573	2.7034942
C	1.1376224	-0.2421616	1.6476110
N	-1.2442363	-0.7753666	2.1297325
H	0.2323760	-0.4436052	3.5933195
O	2.2479038	-0.7849199	1.5456012
O	0.7088525	0.8034695	1.0689782
H	-1.5173181	0.2312196	2.0089447
H	-1.3396249	-1.2029456	1.1666814
H	-1.9027499	-1.2241249	2.7577361
O	-1.5686826	-1.6555374	-0.3781753
H	-0.7663536	-1.7457743	-0.9289002
H	-2.0176196	-0.8741651	-0.7462108
O	0.6384006	-1.6004642	-2.0555514
H	0.8222917	-2.3031674	-2.6823552
H	1.5285125	-1.3366417	-1.6833070
O	2.9176415	-0.7369918	-1.0928324
H	2.8385509	-0.7802676	-0.1163656
H	2.8690961	0.2155050	-1.2596368
O	1.9086062	1.9193713	-1.0005151
H	1.5454562	1.5595636	-0.1494583
H	2.2981972	2.7688816	-0.7863690
O	-2.4761173	0.9014956	-1.1344525
H	-1.6579805	1.0481724	-1.6829970
H	-3.2090931	1.1531163	-1.7002449
O	-1.7957338	1.8158789	1.4759679
H	-2.1769976	1.6831126	0.5916914
H	-0.8375164	1.7732976	1.2994090
O	-0.2558925	1.0553924	-2.5395310
H	0.0540571	0.1354081	-2.5669711
H	0.4749359	1.5257855	-2.1014310

Table 18: Cartesian coordinates (in Angstrom) of the global non–dissociated Gly•$(H_2O)_8$ cluster.

34			
Energy = -894.7050973184			
C	-0.9543281	0.1157210	1.8594656
O	0.1343608	-0.0527363	2.5582871
H	0.6785586	-0.8862815	2.2346319
O	-1.4551217	-0.7159818	1.1061833
C	-1.6061737	1.4598968	2.0935646
H	-2.1682882	1.7146078	1.1987430
H	-2.3252978	1.3218091	2.9075134
N	-0.5989024	2.4870976	2.3540332
H	-1.0462354	3.3657610	2.5805245
H	-0.0440828	2.2121107	3.1552473
O	1.4372253	-0.4649645	-2.6074538
H	0.9167899	0.3532574	-2.6241343
H	1.9807853	-0.3786488	-1.8066307
O	2.6790247	0.0047815	-0.1000323
H	2.1363711	0.8195989	0.0632320
H	3.5929029	0.2937081	-0.0522723
O	1.5978398	-1.8716765	1.6720168
H	2.0994952	-1.3333646	1.0335230
H	1.0562016	-2.4857934	1.1266928
O	-2.1528865	-0.2643766	-1.5874143
H	-2.1031794	-0.4056024	-0.6290552
H	-1.7331843	-1.0588342	-1.9589076
O	-0.2820525	-3.2233999	0.2849361
H	-0.8811843	-2.5356684	0.6074865
H	-0.2888914	-3.0872122	-0.6758591
O	1.1326071	2.1441091	0.1041778
H	0.5740534	2.3626038	0.8779460
H	0.5348607	2.1254903	-0.6608858
O	-0.4305471	-2.3428331	-2.4143492
H	-0.4354281	-2.8979555	-3.1964014
H	0.3235954	-1.7119511	-2.5327008
O	-0.4244895	1.6570629	-2.1843214
H	-0.8070817	2.2828628	-2.8020901
H	-1.1373168	0.9968020	-1.9856961

Table 19: Cartesian coordinates (in Angstrom) of the global zwitterionic Gly•$(H_2O)_8$ cluster.

34
Energy = -894.7062619358

C	2.7282881	0.2233048	0.6188841
H	2.8987273	1.2433780	0.9474454
C	1.3929084	-0.2975956	1.1748364
N	2.7288806	0.1975089	-0.8647903
H	3.5268653	-0.4173629	0.9863901
O	0.8735242	0.3809057	2.0862411
O	0.9771268	-1.3771146	0.6699405
H	3.6469626	0.4104343	-1.2399540
H	2.4065531	-0.7184859	-1.2536197
H	2.0228405	0.9220273	-1.2249968
O	-1.4669110	-2.3425997	1.0823320
H	-1.4304263	-3.2980715	1.1553061
H	-0.5283239	-2.0385225	1.0001313
O	1.4987636	-2.0067819	-1.9636551
H	1.1918361	-2.1192849	-1.0489884
H	0.7556270	-1.5374032	-2.3805370
O	-1.7419236	-0.1280157	2.8237464
H	-1.8598939	-1.0209531	2.4690525
H	-0.7818796	0.0184561	2.7013748
O	-0.1980817	2.6214694	0.6831056
H	0.2161339	2.0118605	1.3144688
H	-1.1417106	2.3994318	0.7503779
O	-2.4883170	-0.6345993	-0.9037037
H	-2.2384474	-1.3320113	-0.2743299
H	-2.6866072	0.1329255	-0.3407008
O	-2.7589313	1.4576536	0.9778581
H	-2.4598716	0.8945189	1.7418402
H	-3.5703161	1.8812803	1.2648602
O	0.8728225	1.8700473	-1.6659958
H	0.2380647	1.2708238	-2.0983080
H	0.4147130	2.2152082	-0.8625260
O	-0.6231709	-0.2497915	-2.7157162
H	-1.3454048	-0.3983143	-2.0456729
H	-1.0704207	-0.2343264	-3.5646969

Table 20: Cartesian coordinates (in Angstrom) of the global non–dissociated Gly•$(H_2O)_9$ cluster.

37
Energy = -971.0443968664

O	-3.2331281	0.0220410	0.8112370
H	-3.3204599	-0.1869693	-0.1431036
H	-4.1237363	0.0077209	1.1669592
O	-1.1837911	-1.9078874	1.4696025
H	-1.8885506	-1.2441128	1.4452455
H	-1.1612585	-2.2569897	0.5498132
C	1.3577428	0.0636742	2.3728447
O	0.4696177	0.7959002	2.7823374
O	1.1921545	-1.1406367	1.8786406
H	0.1978323	-1.3835541	1.7872849
C	2.8148551	0.4660590	2.4368494
N	3.5710924	-0.1204671	1.3304509
H	4.5562115	0.0855113	1.4341854
H	3.4658862	-1.1273527	1.3573637
H	3.1770635	0.1718337	3.4271509
H	2.8570374	1.5500484	2.3794314
O	-1.3987287	2.1220353	1.2122929
H	-0.8311135	1.7075067	1.8814374
H	-2.1162038	1.4810778	1.0838834
O	-1.1507935	-2.6347638	-1.1462761
H	-0.3765692	-2.2483995	-1.5870815
H	-1.8969520	-2.1342821	-1.5042359
O	-3.1120760	-0.6059818	-1.8309437
H	-2.3886153	-0.0441788	-2.2260431
H	-3.8240734	-0.5998901	-2.4735894
O	-1.0823499	0.7223095	-2.8136110
H	-0.3704853	0.0621856	-2.8735188
H	-0.7134239	1.4065610	-2.2276306
O	0.9233201	-1.2103147	-2.4703186
H	1.4968980	-1.5778121	-3.1453469
H	1.5007163	-0.6099474	-1.9291699
O	0.1183206	2.4112361	-0.9236459
H	0.2317657	3.3529509	-1.0676056
H	-0.4597837	2.3349617	-0.1179849
O	2.2952698	0.5918630	-1.1202312
H	2.7542512	0.3856285	-0.2789409
H	1.6520576	1.2924352	-0.9277329

Table 21: Cartesian coordinates (in Angstrom) of the global zwitterionic Gly•$(H_2O)_9$ cluster.

37
Energy = -971.0500178341

O	0.1598044	1.9378334	-2.9881486
H	-0.2024687	2.5700756	-3.6102433
H	-0.5064073	1.8488565	-2.2800854
O	-1.1515042	-1.3592910	3.1532673
H	-0.2540178	-1.0120360	2.9747161
H	-1.6417073	-0.5492588	3.3597046
C	0.9944367	0.7071034	1.4875765
O	0.1442966	1.6345732	1.5614869
O	1.1909317	-0.2432645	2.2779205
H	1.3707186	-1.1151827	-0.3992497
C	1.9209199	0.7260665	0.2623732
N	2.2513729	-0.6859506	-0.0419366
H	2.9952625	-0.7874719	-0.7537412
H	2.4640920	-1.1269233	0.8542031
H	2.8350724	1.2646476	0.4989014
H	1.4559886	1.1761515	-0.6084040
O	-3.4049832	0.3987606	0.5790452
H	-3.1674996	0.7549799	1.4503321
H	-3.1755927	-0.5405459	0.6448984
O	-2.1111247	-2.1867196	0.8468769
H	-1.7445367	-1.9486473	1.7430690
H	-2.5198165	-3.0480546	0.9525261
O	3.7160798	-0.6726417	-2.3352764
H	2.8750125	-0.6455621	-2.8482954
H	4.3328312	-1.1879736	-2.8564658
O	-1.2516450	1.3068736	-0.7674469
H	-2.1377325	1.0692440	-0.4070057
H	-0.7661161	1.6206566	0.0234268
O	-2.1118002	1.2900525	2.9644392
H	-1.2313797	1.4908479	2.5624691
H	-2.2872860	2.0040140	3.5800550
O	-0.2586798	-1.2550199	-0.9784482
H	-0.8754168	-1.7667278	-0.4192217
H	-0.6434710	-0.3508439	-0.9553798
O	1.2447325	-0.5747280	-3.3535133
H	0.6239119	-1.0689064	-2.8021947
H	0.8677218	0.3250131	-3.3722305

Table 22: Cartesian coordinates (in Angstrom) of the global non–dissociated Gly•$(H_2O)_{10}$ cluster.

40			
Energy = -1047.3861931026			
O	-0.0110345	-1.7788304	2.0613423
H	0.1632137	-2.4704547	2.7037439
H	0.8613027	-1.2879909	1.9671707
O	-2.3144860	-0.3383662	2.3320674
H	-2.6313678	-0.3915877	3.2359677
H	-1.4574966	-0.8163536	2.3252964
C	1.9687912	-0.3881278	-1.6000209
O	2.5551232	0.6754858	-1.5058562
O	0.7029039	-0.5279569	-1.9525902
H	0.2442467	0.3859447	-2.0652423
C	2.6559595	-1.7101440	-1.3462975
N	3.7734976	-1.4905920	-0.4338644
H	4.3151526	-0.7031425	-0.7715408
H	4.3818898	-2.2978960	-0.4146831
H	2.9433463	-2.1068800	-2.3254073
H	1.9451430	-2.4069394	-0.9083874
O	-0.2539323	3.2332163	0.1357625
H	-0.3218421	4.1898249	0.1632240
H	-1.0858663	2.8926575	0.5527421
O	-2.5103073	2.1776558	1.0271002
H	-2.4068018	1.3666998	1.5505706
H	-2.9315626	1.8775075	0.2057084
O	2.2456542	-0.5485841	1.8010638
H	2.1949622	0.4123288	1.6142074
H	2.8726009	-0.8988471	1.1363872
O	-0.6073568	1.6330633	-2.1602934
H	-0.3903805	2.2786163	-1.4645373
H	-1.5488829	1.4255812	-2.0149520
O	2.1807896	2.0635130	0.9625899
H	1.3326834	2.5127802	0.8167643
H	2.4597059	1.8403088	0.0653546
O	-3.3163159	-1.3104322	-0.2035381
H	-2.5178269	-1.8402141	-0.4040470
H	-3.1958716	-1.0769316	0.7278686
O	-3.2350340	1.0062294	-1.4443930
H	-4.0055215	1.1121137	-2.0057012
H	-3.3057416	0.0936374	-1.0529984
H	-0.3727764	-1.9083064	-1.1082704
O	-0.8627346	-2.5242112	-0.5465034
H	-0.5138266	-2.3543758	0.3441924

Table 23: Cartesian coordinates (in Angstrom) of the global zwitterionic Gly•$(H_2O)_{10}$ cluster.

40			
Energy = -1047.3921419272			
O	3.0396893	0.6822182	-2.3333303
H	3.9976556	0.7212942	-2.3417760
H	2.8038766	-0.1183850	-1.8024737
O	-1.9490517	-0.4608432	3.2925385
H	-2.2870812	-0.2583662	2.4075591
H	-1.4558231	0.3367902	3.5537203
C	0.9111116	-1.5993650	-0.9189305
O	2.1197212	-1.2672144	-0.7966523
O	0.2285306	-1.7117280	-1.9623525
H	0.6811737	-0.2524716	1.4782767
C	0.2008721	-1.9272223	0.4000127
N	0.9413148	-1.2603365	1.4948883
H	0.7298558	-1.6881189	2.4127719
H	1.9274171	-1.3185322	1.2276547
H	0.2117707	-3.0011779	0.5668892
H	-0.8261129	-1.5792994	0.3995402
O	-0.2003369	1.6618451	3.7449620
H	-0.3258383	2.5347025	4.1202612
H	-0.0007322	1.8047717	2.8014890
O	-2.5686181	0.5114625	0.6588839
H	-2.4672210	0.1632350	-0.2722621
H	-3.3833910	1.0186388	0.6507864
O	-0.7811701	1.6691492	-3.2396375
H	-0.1427402	1.0303516	-3.6616132
H	-1.1178747	2.2123760	-3.9549695
O	1.0487314	2.3379454	-1.1745408
H	1.8314453	1.8843775	-1.5292163
H	0.3934174	2.2615010	-1.8879199
O	0.0430100	1.3168255	1.0650289
H	-0.9039811	1.2002750	0.8605290
H	0.4444813	1.7196918	0.2511023
O	-0.2423442	-2.4925719	3.6182925
H	-0.0931687	-2.6905339	4.5439829
H	-0.9677714	-1.8268466	3.5981110
O	-2.1402839	-0.3239942	-1.7807855
H	-1.4088324	-0.9675181	-1.8617777
H	-1.8298024	0.4218689	-2.3226241
H	1.8203456	0.2014711	-3.7754781
O	0.9584622	-0.1149729	-4.0838633
H	0.7592931	-0.8312932	-3.4470772

Table 24: Optimized Cartesian coordinates (in Angstrom) of the gw10-bb-10 structure, which corresponds to the Gly•$(H_2O)_{10}$ cluster after breaking the water bridge.

40
Energy=-1047.3794721554

O	3.8180076	-0.2895871	-3.2460507
H	4.2266373	-0.9929440	-3.7533138
H	3.3402374	-0.7494083	-2.5247693
O	-1.5930044	-0.4928398	2.9530783
H	-2.1091538	-0.4518191	2.1316997
H	-1.2183490	0.3907282	3.0840201
C	1.0510936	-1.5661314	-1.3084044
O	2.2862134	-1.3339085	-1.2433791
O	0.3168110	-1.6557074	-2.3196355
H	0.9027853	-0.0501200	1.0428284
C	0.3796851	-1.7721566	0.0584889
N	1.1994552	-1.0438827	1.0555351
H	1.1159318	-1.4543523	1.9967833
H	2.1509599	-1.0929766	0.6660971
H	0.3800008	-2.8296965	0.3091367
H	-0.6345660	-1.3935915	0.0781920
O	-0.2943676	2.0585634	3.2215582
H	0.2329063	2.4225971	3.9347029
H	0.2431353	2.1443984	2.4187269
O	-3.0564055	-0.2468755	0.5190307
H	-2.6329630	-0.2199834	-0.3841596
H	-3.9088202	-0.6685589	0.3915081
O	0.1430218	1.9452800	-2.1233568
H	0.6248258	1.4308424	-2.8343684
H	0.0224402	2.8260873	-2.4843669
O	-2.2682660	2.3447011	0.9943233
H	-2.8062641	1.5395432	0.9085481
H	-2.2445913	2.5442380	1.9346290
O	0.2963429	1.5543498	0.5861777
H	-0.6546540	1.7975415	0.6544959
H	0.4914048	1.7537178	-0.3514867
O	0.3226656	-2.3252906	3.3140398
H	0.4772613	-2.5738372	4.2260333
H	-0.4716265	-1.7482282	3.3134946
O	-1.8707889	-0.0760475	-1.8128968
H	-1.2225644	-0.7672739	-2.0594866
H	-1.3689575	0.7441895	-1.9501566
H	2.1966837	0.3132296	-3.8733455
O	1.2297412	0.4168144	-3.9407682
H	0.9070949	-0.4316049	-3.5831834

Table 25: Optimized Cartesian coordinates (in Angstrom) of the gw10-bb-11 structure, which corresponds to the Gly•$(H_2O)_{10}$ cluster after breaking the water bridge.

40
Energy=-1047.3827350157

O	3.4485160	0.4972952	-2.7566438
H	4.4027269	0.4136041	-2.7744247
H	3.1249736	-0.3347203	-2.3487900
O	-1.6943617	-0.5033113	2.9160992
H	-1.9861261	-0.4059633	1.9941623
H	-1.3413657	0.3720230	3.1299537
C	1.1304727	-1.7121534	-1.4139636
O	2.3681055	-1.5213454	-1.3262565
O	0.3886613	-1.6147740	-2.4201804
H	1.1068401	-0.5633464	1.0406523
C	0.4549466	-2.1291885	-0.0990673
N	1.2825486	-1.5922598	1.0063388
H	1.0569588	-2.0266081	1.9141513
H	2.2517256	-1.7207463	0.7047247
H	0.4208988	-3.2131059	-0.0257846
H	-0.5498574	-1.7304590	-0.0154675
O	-0.6355963	2.1917866	2.8175628
H	-0.1172542	2.8006730	3.3470919
H	-0.0570224	1.9212988	2.0686864
O	-2.0700269	0.3120679	0.2482371
H	-2.2253838	0.0416622	-0.6881786
H	-2.5970202	1.1112946	0.4296679
O	-3.0270195	2.6326907	1.3680758
H	-2.2643504	2.6620330	1.9686773
H	-3.7956157	2.6355729	1.9413870
O	1.5147877	2.0329525	-1.5164814
H	2.3543877	1.6443627	-1.8221304
H	0.9151724	1.7718722	-2.2372060
O	0.4954596	1.0129318	0.6904879
H	-0.4240085	0.7992116	0.4065247
H	0.9231428	1.4263289	-0.1116214
O	0.0097972	-2.5514817	3.2176798
H	0.0022469	-2.9484692	4.0888860
H	-0.6741747	-1.8444751	3.2243671
O	-2.1371290	-0.5446196	-2.2869419
H	-1.3391534	-1.1092116	-2.3194744
H	-1.9037048	0.1508759	-2.9125642
H	0.6504197	0.9620342	-4.4352598
O	0.1300213	0.7848544	-3.6482054
H	0.4063610	-0.1111874	-3.3647721

Table 26: Optimized Cartesian coordinates (in Angstrom) of the gw10-bb-12 structure, which corresponds to the Gly•$(H_2O)_{10}$ cluster after breaking the water bridge.

40
Energy=-1047.3840698104

O	2.9862676	0.8192339	-3.2416858
H	3.9174160	0.7359647	-3.4525842
H	2.7883982	0.0631233	-2.6465023
O	-2.3667463	-0.1392340	2.3917118
H	-2.5583693	0.1231702	1.4771595
H	-1.8058484	0.5708272	2.7355753
C	1.0594221	-1.4106798	-1.2712154
O	2.2334319	-0.9747290	-1.3681437
O	0.2523974	-1.6843140	-2.1922749
H	0.9391122	0.2559453	0.8591110
C	0.5716257	-1.6252409	0.1688310
N	1.3359211	-0.6894436	1.0233830
H	1.3005411	-0.8886880	2.0471538
H	2.2845429	-0.6882378	0.6392574
H	0.7662356	-2.6466029	0.4848648
H	-0.4883799	-1.4212511	0.2730197
O	-0.2801904	1.7159757	3.1112145
H	-0.3199395	2.5497072	3.5842556
H	-0.0861086	1.9472721	2.1809007
O	-2.5553318	0.8717089	-0.2344091
H	-2.4787886	0.3237227	-1.0637381
H	-3.2843797	1.4754475	-0.3932712
O	1.0020758	-0.8757167	3.7285619
H	0.2433862	-1.4899333	3.7555333
H	0.6093418	0.0028033	3.8217195
O	0.9771205	2.3323557	-1.9631709
H	1.8844292	2.0995564	-2.2124154
H	0.4765781	1.7727831	-2.5852931
O	0.0091958	1.6761618	0.4161791
H	-0.9108450	1.4801411	0.1499521
H	0.4347673	2.0064021	-0.4184746
O	-1.1587765	-2.4321266	3.1420538
H	-1.7386404	-3.0173692	3.6316670
H	-1.7232280	-1.6887544	2.8423899
O	-2.2224343	-0.5949885	-2.3895168
H	-1.4408835	-1.1658811	-2.2370505
H	-1.9437321	-0.0768181	-3.1537437
H	0.9000131	0.6312655	-4.3623805
O	0.0920486	0.4471208	-3.8716629
H	0.2983541	-0.3906793	-3.4069615

Table 27: Optimized Cartesian coordinates (in Angstrom) of the gw10-bb-13 structure, which corresponds to the Gly•$(H_2O)_{10}$ cluster after breaking the water bridge.

40
Energy=-1047.3823050270

O	3.1976480	0.8563518	-2.7336079
H	4.1430109	0.8605593	-2.5773313
H	2.8768848	0.0190749	-2.3357824
O	-2.1113357	-0.1408503	2.6536580
H	-2.4002918	0.0080930	1.7402046
H	-1.6213638	0.6629564	2.8905327
C	0.8770080	-1.4660420	-1.5029493
O	2.0883992	-1.1892181	-1.3592754
O	0.1774002	-1.4369269	-2.5474576
H	0.6375861	-0.2840888	0.9232902
C	0.1633270	-1.9153963	-0.2200822
N	0.8597968	-1.2970759	0.9252568
H	0.5901257	-1.7004627	1.8292440
H	1.8634781	-1.3706564	0.7536600
H	0.2172880	-2.9978366	-0.1323237
H	-0.8768405	-1.6073655	-0.2068072
O	-0.2397184	1.9700799	3.0028385
H	-0.2879475	2.8945809	3.2532826
H	-0.0599330	1.9548984	2.0373080
O	-2.6563020	0.6259347	-0.0492219
H	-2.5953807	0.2082256	-0.9513872
H	-3.4241715	1.2004626	-0.0898865
O	1.6454550	-0.1707268	3.4878917
H	1.0653864	-0.8147302	3.9066692
H	1.1386439	0.6512893	3.5272667
O	1.0563876	2.2909699	-1.7727637
H	1.9412401	1.9442921	-1.9943496
H	0.5282564	1.9568730	-2.5179482
O	-0.0062749	1.3128826	0.4247485
H	-0.9441785	1.2183984	0.1770389
H	0.4392844	1.7027987	-0.3801283
O	-0.4830797	-2.1649408	3.2669981
H	-0.9174345	-2.9477767	3.6093065
H	-1.1949882	-1.5057931	3.0953310
O	-2.3315984	-0.4536238	-2.4321950
H	-1.5108077	-0.9939578	-2.4353070
H	-2.1135226	0.2126211	-3.0956312
H	0.2931338	1.0280380	-4.7120284
O	-0.1794219	0.8704249	-3.8916308
H	0.1548508	0.0076629	-3.5664311

Table 28: Optimized Cartesian coordinates (in Angstrom) of the gw10-bb-14 structure, which corresponds to the Gly•$(H_2O)_{10}$ cluster after breaking the water bridge.

40
Energy=-1047.3778527322

O	3.2908798	0.9880795	-2.6390925
H	4.2394848	0.8709465	-2.5729345
H	2.9045546	0.1788839	-2.2387905
O	-2.1839270	0.0360426	2.6472636
H	-2.4368162	0.2649929	1.7400551
H	-1.6380756	0.7880084	2.9413413
C	0.8098943	-1.1348282	-1.4119104
O	2.0397999	-0.9577743	-1.2544577
O	0.1302712	-1.0290805	-2.4647404
H	0.7077349	-0.0154479	1.0260607
C	0.0471180	-1.5467968	-0.1475376
N	0.8192301	-1.0486926	1.0144006
H	0.5105161	-1.4587361	1.9039705
H	1.7976036	-1.2577919	0.8079560
H	-0.0145132	-2.6284439	-0.0785306
H	-0.9469962	-1.1136639	-0.1193927
O	-0.2649282	1.9400004	3.2606116
H	-0.3162852	2.8207435	3.6351530
H	0.0332582	2.0608859	2.3385459
O	-2.5024078	1.1324603	0.0242575
H	-2.4845655	0.7704367	-0.9041375
H	-3.2074029	1.7839611	0.0259247
O	0.7639766	-3.9298035	1.8505542
H	0.6666235	-4.8830053	1.8583432
H	0.1056707	-3.5975177	2.4751733
O	1.3346314	2.5984449	-1.5470131
H	2.1825311	2.1841894	-1.7909098
H	0.7755916	2.3306845	-2.2967832
O	0.1792672	1.6162944	0.6139011
H	-0.7568851	1.5842897	0.3426948
H	0.6611312	2.0107322	-0.1649567
O	-0.6126078	-2.0000633	3.3085721
H	-0.3976851	-1.8418971	4.2304062
H	-1.3011692	-1.3251548	3.0888859
O	-2.2903606	0.1529776	-2.4104096
H	-1.5198758	-0.4570600	-2.4025754
H	-1.9917593	0.8182877	-3.0425257
H	0.5769374	1.4985095	-4.4990857
O	0.0248650	1.3479915	-3.7282779
H	0.2646895	0.4479145	-3.4200098

Table 29: Optimized Cartesian coordinates (in Angstrom) of the gw10-bb-15 structure, which corresponds to the Gly•$(H_2O)_{10}$ cluster after breaking the water bridge.

40
Energy=-1047.3846351746

O	2.9054132	1.0812344	-2.7227243
H	3.8614122	1.1189087	-2.6677135
H	2.6527976	0.2708691	-2.2328705
O	-2.5103507	0.0188085	2.8631145
H	-2.7578922	0.1859698	1.9416300
H	-1.9360334	0.7695185	3.0976528
C	0.8263634	-1.2880325	-1.1610206
O	2.0316693	-0.9260079	-1.1061270
O	0.0757116	-1.2699101	-2.1634242
H	0.5744320	-0.1314208	1.1969313
C	0.2078752	-1.8346096	0.1301935
N	0.7501413	-1.1454884	1.3238270
H	0.2504094	-1.4825408	2.1689720
H	1.7617712	-1.3198744	1.4122290
H	0.4203261	-2.8983381	0.2135967
H	-0.8687168	-1.6984694	0.1211231
O	-0.5451482	1.9518225	3.2508466
H	-0.5710071	2.8590753	3.5583501
H	-0.2687774	1.9961011	2.3159489
O	-2.8009573	0.8320875	0.1272319
H	-2.7673159	0.3555710	-0.7435470
H	-3.4845959	1.4978662	0.0244974
O	3.4998565	-1.6021685	1.0237431
H	4.0137914	-2.4079132	0.9498772
H	3.1712893	-1.4066044	0.1205877
O	0.8057227	2.4977436	-1.6087075
H	1.6875221	2.1892670	-1.8834999
H	0.2515361	2.1269392	-2.3155131
O	-0.1227992	1.4054456	0.6256778
H	-1.0652475	1.3033145	0.3946600
H	0.2860837	1.8337843	-0.1726460
O	-0.9753275	-2.1251102	3.2088843
H	-0.9144239	-2.3518565	4.1380967
H	-1.6318944	-1.3889650	3.1555247
O	-2.5158982	-0.4267413	-2.1876793
H	-1.6809701	-0.9319019	-2.1185672
H	-2.2950801	0.1967567	-2.8908612
H	0.1035213	1.0922723	-4.4566782
O	-0.4043348	0.9340851	-3.6574905
H	-0.0208747	0.1185122	-3.2741261

Table 30: Optimized Cartesian coordinates (in Angstrom) of the gw10-bb-17 structure, which corresponds to the Gly•$(H_2O)_{10}$ cluster after breaking the water bridge.

40
Energy=-1047.3770610669

O	2.7213174	0.9489828	-2.6003126
H	3.5068504	0.5167715	-2.9527704
H	2.3501343	0.2440116	-2.0405569
O	-2.1879374	-0.1886121	3.1962656
H	-2.5487761	0.0471112	2.3303361
H	-1.6867136	0.5978955	3.4764571
C	0.4887704	-1.4022151	-1.0151146
O	1.7217431	-1.1401467	-0.9813632
O	-0.2594044	-1.4847494	-2.0146317
H	0.4690107	-0.0148024	1.3883178
C	-0.1534857	-1.6672796	0.3500286
N	0.6860187	-1.0333753	1.3912973
H	0.5014975	-1.4501755	2.3200666
H	1.6523668	-1.1429922	1.0738161
H	-0.1960167	-2.7380207	0.5325737
H	-1.1570764	-1.2602555	0.4065577
O	-0.4107527	1.8847538	3.7085803
H	-0.5023204	2.7507748	4.1088090
H	-0.1914154	2.0445852	2.7731668
O	-2.8147181	0.9110726	0.5773189
H	-2.7817625	0.5717597	-0.3540947
H	-3.5861782	1.4813808	0.6104779
O	3.8606715	-1.7741295	-2.7841392
H	3.5964927	-2.3571032	-3.4977781
H	3.0932726	-1.7630158	-2.1925671
O	0.7636131	2.5103012	-1.2761668
H	1.6887702	2.3543426	-1.5088577
H	0.3033832	2.0202085	-1.9831382
O	-0.1603023	1.5653372	1.0219840
H	-1.1132400	1.4880098	0.8270852
H	0.2378530	1.9614801	0.2038452
O	-0.4905591	-2.2389410	3.5237654
H	-0.3500066	-2.4475456	4.4485340
H	-1.2142774	-1.5733858	3.5035196
O	-2.5458290	-0.0154533	-1.8950154
H	-1.8431165	-0.6970964	-1.9281229
H	-2.2496927	0.6241490	-2.5514229
H	0.8754306	1.0244505	-3.6774508
O	-0.0463454	0.8796653	-3.4252451
H	-0.0272696	-0.0377485	-3.0940546

Table 31: Optimized Cartesian coordinates (in Angstrom) of the gw10-bb-18 structure, which corresponds to the Gly•$(H_2O)_{10}$ cluster after breaking the water bridge.

40
Energy=-1047.3774988549

O	1.6574274	2.0869001	-1.8760475
H	2.5236250	2.4477007	-2.0752652
H	1.7468204	1.1048696	-1.9444087
O	-2.1891229	0.6959804	2.7954613
H	-2.4191434	1.0441158	1.9210274
H	-1.4232429	1.2281553	3.0711555
C	0.3447986	-0.9377006	-1.7001018
O	1.5579119	-0.5479594	-1.6621004
O	-0.4468320	-0.8334651	-2.6514256
H	0.5132518	-0.1059281	0.7894314
C	-0.1993204	-1.6027869	-0.4345166
N	0.5111956	-1.1390119	0.7818789
H	0.0082749	-1.4931676	1.6196791
H	1.4797542	-1.4641561	0.7817480
H	-0.0834938	-2.6812901	-0.4944862
H	-1.2521980	-1.3677155	-0.3154672
O	0.2438294	2.0166824	3.2398861
H	0.4116460	2.8808999	3.6186165
H	0.4550204	2.0983062	2.2931476
O	-2.3836692	1.9059222	0.1878046
H	-2.5291191	1.5058964	-0.7166129
H	-2.9164745	2.7042212	0.1964558
O	3.1941212	-1.9199136	-0.1052660
H	4.0866563	-1.5741164	-0.0607483
H	2.7254091	-1.4014640	-0.8037815
O	1.5919169	-3.9242657	0.9017894
H	1.6618099	-4.8634052	0.7253828
H	2.3721480	-3.5270516	0.4895924
O	0.3179366	1.7071164	0.5227599
H	-0.6191180	1.9119230	0.3257838
H	0.8278202	1.9921477	-0.2589705
O	-1.3185732	-1.8263830	2.6672297
H	-1.3075316	-2.2642301	3.5192042
H	-1.7270287	-0.9415132	2.8130512
O	-2.6033986	0.8959299	-2.2168908
H	-2.1470994	0.0421440	-2.2898165
H	-2.0405897	1.4364037	-2.8048978
H	0.2014971	2.1487489	-3.2969466
O	-0.5087177	1.7548918	-3.8197161
H	-0.3181979	0.8065686	-3.7336194

Table 32: Optimized Cartesian coordinates (in Angstrom) of the gw10-bb-19 structure, which corresponds to the Gly•$(H_2O)_{10}$ cluster after breaking the water bridge.

40
Energy=-1047.3801887192

O	1.4127182	1.3743854	-1.4067362
H	2.2139111	1.6695876	-1.8850034
H	1.6433646	0.4714173	-1.1201954
O	-2.4404199	0.3416657	3.0016309
H	-2.7003587	0.4235904	2.0720052
H	-1.9411257	1.1559058	3.1883349
C	0.5275071	-1.7389661	-0.6003403
O	1.7014847	-1.2578880	-0.5586361
O	-0.0946123	-2.1715605	-1.5866354
H	0.2905072	0.0777736	1.4831061
C	-0.1957297	-1.7870708	0.7503896
N	0.5124671	-0.9115666	1.7135898
H	0.2305803	-1.1316459	2.6854626
H	1.5105433	-1.0354931	1.5369830
H	-0.1957288	-2.8041939	1.1330569
H	-1.2224941	-1.4485812	0.6587864
O	-0.6387962	2.4408524	3.3045486
H	-0.7327565	3.3672029	3.5317298
H	-0.3412715	2.4223016	2.3784509
O	-2.7574375	0.8968666	0.1918188
H	-2.6942735	0.2863161	-0.5965407
H	-3.5064281	1.4678150	0.0054493
O	3.2102864	-1.2189204	-2.8746764
H	2.6921040	-1.6237931	-3.5734563
H	2.6796727	-1.3692577	-2.0663916
O	3.7158893	1.4934833	-2.8509316
H	3.8170010	1.8587155	-3.7312078
H	3.6338868	0.5273948	-2.9822620
O	-0.1695043	1.6184198	0.7493260
H	-1.0811620	1.5130724	0.4133402
H	0.4049053	1.7588343	-0.0337781
O	-0.8904829	-1.6403625	3.9180431
H	-0.8482794	-1.6553508	4.8753707
H	-1.5783116	-0.9759193	3.6872361
O	-2.4508341	-0.6662392	-1.8857387
H	-1.9098599	-1.4510136	-1.6997704
H	-1.8728917	-0.2086952	-2.5274026
H	0.2969775	0.6678497	-2.8585750
O	-0.2442137	0.0655968	-3.3928477
H	0.0131655	-0.8025292	-3.0475333

Table 33: Optimized Cartesian coordinates (in Angstrom) of the gw10-bb-1 structure, which corresponds to the Gly•$(H_2O)_{10}$ cluster after breaking the water bridge.

40
Energy=-1047.3792864951

O	2.1970721	1.2973788	-1.1263676
H	3.0650914	1.5436934	-1.4593251
H	2.2551985	0.3236788	-1.0398826
O	-1.9393568	0.2571241	3.1680280
H	-2.1710504	0.5475157	2.2723207
H	-1.2859090	0.9098793	3.4732826
C	0.6484444	-1.5869783	-0.7790738
O	1.8874601	-1.3755378	-0.6660446
O	-0.0445031	-1.5975356	-1.8194828
H	0.7260889	-0.3201109	1.6076329
C	-0.0893535	-1.8658697	0.5343369
N	0.7349930	-1.3573561	1.6554333
H	0.3669626	-1.6880357	2.5662266
H	1.6958198	-1.6455350	1.4708930
H	-0.2369104	-2.9353041	0.6599585
H	-1.0562630	-1.3742503	0.5597213
O	0.2509431	1.8843576	3.7409078
H	0.3297300	2.7683666	4.1027391
H	0.5338905	1.9498855	2.8125425
O	-2.0755318	1.2814139	0.4929803
H	-2.2412338	0.7259386	-0.3281847
H	-2.6250229	2.0606536	0.3794893
O	-1.8130036	1.3767072	-3.7868729
H	-0.8716857	1.1051825	-3.8183339
H	-2.1421979	1.2402941	-4.6766537
O	3.6072166	-0.7138009	-2.9517972
H	3.1124365	-1.2208302	-2.2942505
H	2.9286011	-0.4889347	-3.5957625
O	0.5734147	1.3746036	1.0784916
H	-0.3397717	1.4789463	0.7371073
H	1.1780564	1.5576694	0.3338381
O	-0.8744378	-2.1375484	3.6875380
H	-0.8815577	-2.3478907	4.6224209
H	-1.3968061	-1.3087349	3.5899880
O	-2.4205727	-0.1977657	-1.6153642
H	-1.6803231	-0.8265135	-1.7097908
H	-2.3506462	0.3517720	-2.4213522
H	1.1855154	0.9424521	-2.8618264
O	0.7402897	0.4154502	-3.5405677
H	0.5189124	-0.4044307	-3.0549431

Table 34: Optimized Cartesian coordinates (in Angstrom) of the gw10-bb-21 structure, which corresponds to the Gly•$(H_2O)_{10}$ cluster after breaking the water bridge.

40
Energy=-1047.3743385797

O	1.7220961	1.9376313	-2.1345956
H	2.5650177	2.3622770	-2.3062462
H	1.9243593	0.9851874	-1.9702512
O	-2.2309740	0.3960272	2.1929628
H	-2.5128349	0.6247660	1.2938421
H	-1.6931086	1.1557739	2.4734477
C	0.6556765	-1.0650260	-1.4629079
O	1.8468842	-0.6179247	-1.3938749
O	-0.0120097	-1.2851096	-2.4864264
H	0.4863389	0.4158148	0.7744570
C	-0.0280176	-1.3633068	-0.1260382
N	0.6103141	-0.5908990	0.9711377
H	0.1943085	-0.8340283	1.8802457
H	1.6122938	-0.8038594	1.0013018
H	0.0563355	-2.4214284	0.1106689
H	-1.0765196	-1.0862779	-0.1683938
O	-0.3051191	2.3520491	2.7435858
H	-0.3527194	3.2088445	3.1706918
H	-0.0502250	2.5275563	1.8212398
O	-2.5523799	1.4434116	-0.4548708
H	-2.5330578	0.9450190	-1.3253048
H	-3.2826726	2.0612007	-0.5367264
O	3.1202349	-1.8410905	0.6284222
H	2.8868540	-1.4913254	-0.2595888
H	4.0768279	-1.8135194	0.6867826
O	1.0527260	-3.7195391	1.7969242
H	0.5657479	-3.1893134	2.4353154
H	1.8596815	-3.2277478	1.6077884
O	0.0671566	2.0324934	0.0740077
H	-0.8538554	1.9721727	-0.2498356
H	0.6377944	2.1835506	-0.7038923
O	-0.7629925	-1.6210742	3.2136703
H	-0.7078669	-1.4929857	4.1630429
H	-1.4846447	-1.0253300	2.9192709
O	-2.3532752	0.1594185	-2.7073933
H	-1.7746232	-0.6099905	-2.5645359
H	-1.7940983	0.6762126	-3.3179297
H	0.4564219	1.5555690	-3.6907563
O	-0.1515718	0.9967403	-4.1912584
H	0.1154964	0.1080602	-3.9079792

Table 35: Optimized Cartesian coordinates (in Angstrom) of the gw10-bb-22 structure, which corresponds to the Gly•$(H_2O)_{10}$ cluster after breaking the water bridge.

40
Energy=-1047.3784098603

O	2.4153260	0.3789042	-0.5760169
H	3.2933248	0.3792190	-1.0071867
H	2.2170382	-0.5484389	-0.3245702
O	-3.1195402	0.5030937	2.0498482
H	-3.0938049	0.2855096	1.0981808
H	-2.6280810	1.3332698	2.1533126
C	0.0098849	-1.9168171	-0.0159177
O	1.2458373	-1.8804957	0.2054105
O	-0.5987632	-1.8700384	-1.1140058
H	-0.1934449	-0.1132562	1.8015185
C	-0.8480947	-1.9874833	1.2528355
N	-0.2297069	-1.0539567	2.2305957
H	-0.7759323	-1.0293232	3.1120380
H	0.7377973	-1.3466517	2.3556632
H	-0.8257045	-2.9886758	1.6747038
H	-1.8714932	-1.6776882	1.0902424
O	-1.3137398	2.5808752	2.6226102
H	-1.3871482	3.5363813	2.6314065
H	-0.6056759	2.3770045	1.9882301
O	2.9233898	-0.4177076	-4.2978311
H	2.8265501	0.0599242	-5.1228605
H	2.0424383	-0.3860470	-3.8788470
O	-1.0439952	1.7296326	-1.7452892
H	-0.4507056	1.1180489	-2.2446724
H	-1.0732890	2.5430638	-2.2525805
O	0.2211467	1.3487241	0.7317184
H	1.1251372	1.2007558	0.3906599
H	-0.2924181	1.5318454	-0.0783043
O	4.5941510	0.2978085	-2.2280884
H	5.2772437	-0.3699292	-2.1478069
H	4.0995243	0.0538119	-3.0351156
O	-2.2561176	-1.0737118	4.0181272
H	-2.4872016	-0.7291150	4.8820318
H	-2.7333051	-0.5083449	3.3662916
O	-2.8284637	-0.1985081	-0.6407074
H	-2.1891085	-0.8939994	-0.8829248
H	-2.4920626	0.5672063	-1.1254670
H	1.3469792	0.1475370	-1.9820130
O	0.6961705	-0.0936880	-2.6759227
H	0.2658573	-0.8887396	-2.2792969

Table 36: Optimized Cartesian coordinates (in Angstrom) of the gw10-bb-23 structure, which corresponds to the Gly•$(H_2O)_{10}$ cluster after breaking the water bridge.

40
Energy=-1047.3798348856

O	2.9149935	0.4537038	-1.0413473
H	3.8593365	0.5689272	-1.1645478
H	2.7868942	-0.4872045	-0.7552130
O	-2.0796536	-0.3093458	2.5881535
H	-2.2091317	-0.4952446	1.6375013
H	-1.7143594	0.5883975	2.6434999
C	0.9611644	-2.1192072	-0.1101222
O	2.1949820	-1.8633343	-0.0800851
O	0.1893938	-2.1551306	-1.0960108
H	0.8158383	-0.4581569	1.8349675
C	0.3486898	-2.3832744	1.2687134
N	0.9708702	-1.4130274	2.2066399
H	0.5641691	-1.5071463	3.1572952
H	1.9767676	-1.5652515	2.1804001
H	0.5844992	-3.3888163	1.6069920
H	-0.7217937	-2.2295645	1.2850954
O	-0.5879323	2.0521217	2.9377283
H	-0.8930415	2.9596506	2.8886504
H	0.0626247	1.9596814	2.2218742
O	-1.4836059	3.1446750	-3.1967129
H	-1.1642124	2.5308295	-3.8868493
H	-1.0463685	3.9762276	-3.3856485
O	-0.8494858	1.3471148	-1.2259518
H	-0.3076301	0.8191024	-1.8485039
H	-1.1254445	2.1167727	-1.7614295
O	0.8745362	1.0795577	0.8301548
H	1.7078164	1.0762886	0.3286713
H	0.1988837	1.2460252	0.1317297
O	-0.4107387	1.2304339	-4.8615589
H	0.0466235	0.6178816	-4.2569871
H	-0.9477563	0.6711511	-5.4250061
O	-0.7036737	-1.8125711	4.2874168
H	-0.8300145	-1.5418110	5.1980307
H	-1.3563925	-1.2946855	3.7581339
O	-2.2012868	-0.8512211	-0.1421022
H	-1.5496738	-1.4521648	-0.5399202
H	-1.9796432	-0.0052419	-0.5645035
H	1.6593795	0.1111703	-2.4736426
O	0.8028495	-0.1826676	-2.8217799
H	0.6415267	-1.0346453	-2.3537256

Table 37: Optimized Cartesian coordinates (in Angstrom) of the gw10-bb-24 structure, which corresponds to the Gly•$(H_2O)_{10}$ cluster after breaking the water bridge.

40
Energy=-1047.3806637416

O	2.1446613	-0.4029284	-3.0166478
H	2.9983983	-0.7514985	-3.2806099
H	1.9144869	-0.8853860	-2.1707784
O	-2.4589859	-0.4475211	2.6571654
H	-2.6151762	-0.6386512	1.7152506
H	-2.3401135	0.5186378	2.6803206
C	0.4127039	-2.0327328	-0.4467268
O	1.5324846	-1.5345023	-0.7411234
O	-0.5091952	-2.4118597	-1.2041014
H	0.6075088	-0.2082702	1.4277768
C	0.1574262	-2.1930038	1.0519394
N	0.9073896	-1.1453253	1.7848850
H	0.7005676	-1.2117905	2.7961829
H	1.8949883	-1.2347741	1.5622927
H	0.4978936	-3.1698330	1.3864914
H	-0.8924821	-2.0824129	1.2890279
O	-1.7403611	2.2351969	2.5153685
H	-2.3221257	2.8862845	2.1194590
H	-1.0801791	2.0282566	1.8271792
O	2.2927960	2.6908227	-0.0687893
H	2.1693903	2.6441027	-1.0355243
H	2.3880912	3.6235379	0.1314117
O	-0.9712169	1.0944206	-1.7677394
H	-0.8948033	0.3443702	-2.4094781
H	-0.4000657	1.7649993	-2.1634711
O	0.1053271	1.2560323	0.7146279
H	0.8919858	1.8037949	0.5078814
H	-0.3064061	1.0903672	-0.1662243
O	1.5963321	2.2177966	-2.6932691
H	1.8631070	1.2819513	-2.8510271
H	1.8351504	2.6876662	-3.4947478
O	-0.4649675	-1.5145965	4.0803945
H	-0.5484335	-1.2783136	5.0050707
H	-1.2748681	-1.1615590	3.6384027
O	-2.6267505	-0.8472085	-0.1413561
H	-2.0568826	-1.5096461	-0.5697448
H	-2.4773703	-0.0530015	-0.6660193
H	0.2933854	-0.8476713	-3.7270316
O	-0.6346434	-0.9564033	-3.4841054
H	-0.5890478	-1.6493486	-2.7926130

Table 38: Optimized Cartesian coordinates (in Angstrom) of the gw10-bb-25 structure, which corresponds to the Gly•$(H_2O)_{10}$ cluster after breaking the water bridge.

40
Energy=-1047.3885719514

O	2.0857143	0.8365137	-3.0357883
H	2.9358517	0.8560912	-3.4787377
H	2.0592144	-0.0153191	-2.5341851
O	-2.9187632	-0.0089530	2.5015867
H	-3.0499785	-0.0861450	1.5476110
H	-2.2530299	0.6927138	2.6081098
C	0.7077461	-1.6388580	-1.0917141
O	1.8737692	-1.2760159	-1.4187538
O	-0.3383550	-1.5484494	-1.7749539
H	-1.0478666	-0.8808116	0.6421962
C	0.5266155	-2.2118196	0.3203390
N	-0.1957515	-1.2014978	1.1342970
H	-0.4881775	-1.5777363	2.0542136
H	0.3962005	-0.3528307	1.2621657
H	1.4772805	-2.4175682	0.8000935
H	-0.0818204	-3.1103614	0.2775853
O	-0.7611179	1.7089028	2.9852452
H	0.0826572	1.6164814	2.5083073
H	-0.8389860	2.6449019	3.1763880
O	1.3380217	1.0884405	1.3151876
H	2.2248742	0.6894715	1.2548079
H	1.2221956	1.5970338	0.4725422
O	-1.7053722	1.9103244	-1.8871311
H	-1.3559712	1.3848499	-2.6593050
H	-2.3191608	2.5481381	-2.2575065
O	0.9402094	2.4025578	-0.9660073
H	1.4227666	1.9920834	-1.7022655
H	0.0104629	2.3743681	-1.2441639
O	3.3749835	-0.6403356	0.7379025
H	2.9653092	-0.9209313	-0.1106586
H	4.3223598	-0.6630060	0.5958440
O	-1.5068784	-2.1340218	3.3697273
H	-1.3287804	-2.1111426	4.3114361
H	-2.1551333	-1.4136561	3.2043830
O	-2.4406039	-0.3178094	-0.3808263
H	-2.0594805	-0.9416296	-1.0198378
H	-2.3017127	0.5414409	-0.8235997
H	0.3031077	0.6550838	-3.8201311
O	-0.6147718	0.3660364	-3.7127627
H	-0.5076282	-0.4365352	-3.1616406

Table 39: Optimized Cartesian coordinates (in Angstrom) of the gw10-bb-26 structure, which corresponds to the Gly•$(H_2O)_{10}$ cluster after breaking the water bridge.

40
Energy=-1047.3920556603

O	2.1820903	0.9486584	-2.8235056
H	3.0949941	0.9860867	-3.1145102
H	2.1137027	0.1469888	-2.2514696
O	-2.6267568	-0.4225239	2.4153640
H	-2.7258927	-0.3029073	1.4602825
H	-2.3485691	0.4531912	2.7396796
C	0.6308877	-1.4632501	-0.8996005
O	1.8182519	-1.0838326	-1.1088939
O	-0.3266696	-1.4444142	-1.7048838
H	0.8125669	-0.2430810	1.3946216
C	0.3208415	-2.0232356	0.4922343
N	1.0040427	-1.2520674	1.5597729
H	0.5814392	-1.5174691	2.4672518
H	2.0178716	-1.4293361	1.5356883
H	0.6493492	-3.0587601	0.5483951
H	-0.7459802	-1.9895938	0.6829441
O	-1.3421659	1.8979848	3.2161880
H	-1.6582709	2.8009699	3.2749330
H	-0.7732057	1.8729956	2.4238675
O	-0.0249345	1.2201489	0.9078985
H	0.3634574	1.8055161	0.2103021
H	-0.8250017	0.8625061	0.4660599
O	-1.7955513	2.0354694	-2.4219482
H	-1.3235963	1.4165388	-3.0405770
H	-2.3991476	2.5408212	-2.9701816
O	0.7173487	2.7203829	-1.1762351
H	1.3227796	2.2333276	-1.7596143
H	-0.1287152	2.7073969	-1.6496894
O	3.6290046	-1.7048424	0.7728068
H	3.1457529	-1.5309982	-0.0632169
H	4.1690431	-2.4803977	0.6131331
O	-0.7577518	-2.0347753	3.4882963
H	-0.8403267	-1.9978934	4.4425658
H	-1.5129719	-1.5056034	3.1405467
O	-2.1875753	0.1172690	-0.4092882
H	-1.7062364	-0.5653866	-0.9172682
H	-2.3247494	0.8226462	-1.0663784
H	0.5345254	0.6092699	-3.8270595
O	-0.3835964	0.3022638	-3.8359601
H	-0.3502842	-0.4500640	-3.2125515

Table 40: Optimized Cartesian coordinates (in Angstrom) of the gw10-bb-27 structure, which corresponds to the Gly•$(H_2O)_{10}$ cluster after breaking the water bridge.

40
Energy=-1047.3852251191

O	2.1500228	1.4998814	-2.0148471
H	3.0744833	1.7549026	-2.0426680
H	2.1443273	0.5131849	-1.9606864
O	-2.3789500	-0.3732087	1.5097187
H	-2.5744664	-0.4172275	0.5517471
H	-2.1951862	0.5528467	1.7038863
C	0.5861954	-1.4498862	-1.5257573
O	1.7993307	-1.0847770	-1.6009670
O	-0.2892019	-1.3294801	-2.4066294
H	0.3656480	-0.2704691	0.7507095
C	0.1620717	-2.0870572	-0.1983974
N	0.6163535	-1.2481204	0.9378612
H	0.1411350	-1.5557326	1.8193132
H	1.6390426	-1.3123968	1.0391442
H	0.6160640	-3.0700419	-0.0955077
H	-0.9158457	-2.1801932	-0.1395131
O	-0.9805239	2.1374722	2.2513481
H	-1.2408720	3.0522401	2.3737111
H	-0.4885890	2.1036246	1.4034687
O	0.5205987	0.3611099	3.7717856
H	1.1040424	0.7543541	4.4223032
H	0.0132816	1.1011232	3.3966551
O	-1.7429049	1.9906654	-2.0770402
H	-1.1626512	1.6893675	-2.8286267
H	-2.1138292	2.8320065	-2.3493605
O	0.1286750	1.5046374	-0.0987228
H	0.9411089	1.6730373	-0.6108908
H	-0.5844184	1.6877729	-0.7445014
O	3.3725452	-1.5158037	0.5062652
H	2.9745176	-1.4532991	-0.3899079
H	3.9486468	-2.2817753	0.4910637
O	-0.8499946	-2.0013657	3.1236302
H	-0.4842761	-1.3122110	3.6973443
H	-1.6063468	-1.5564436	2.6994473
O	-2.7207951	-0.5367807	-1.2232258
H	-1.9857077	-0.9644782	-1.6972690
H	-2.6813653	0.3679403	-1.5640302
H	0.8060917	1.3332318	-3.5175687
O	-0.0479365	1.0103238	-3.8353898
H	-0.0603212	0.0810254	-3.5278956

Table 41: Optimized Cartesian coordinates (in Angstrom) of the gw10-bb-28 structure, which corresponds to the Gly•$(H_2O)_{10}$ cluster after breaking the water bridge.

40
Energy=-1047.3844505167

O	1.9857857	1.6872920	-1.8190365
H	2.9132135	1.9292590	-1.8550286
H	1.9640022	0.7049889	-1.7162975
O	-2.8810645	-0.0459741	1.8861464
H	-2.9579374	-0.1156698	0.9136329
H	-2.4652305	0.8131104	2.0587212
C	0.3494830	-1.2032500	-1.2173698
O	1.5733241	-0.8784213	-1.3286645
O	-0.5407209	-1.0910768	-2.0818903
H	0.1825849	0.1446649	0.9290764
C	-0.0496885	-1.7570943	0.1516483
N	0.4080605	-0.8205793	1.2114190
H	-0.0838208	-1.0536617	2.0959562
H	1.4294583	-0.8937567	1.3625206
H	0.4284082	-2.7193664	0.3205846
H	-1.1247178	-1.8646303	0.2356578
O	-1.2423856	2.1721195	2.5242772
H	-1.4770416	3.0550440	2.8138811
H	-0.7008361	2.2940447	1.7258319
O	3.1419726	-1.1680427	1.7464879
H	3.4325232	-1.6270050	2.5365938
H	3.4659032	-1.7094885	0.9973833
O	-1.9303982	2.2685033	-1.8383303
H	-1.3633093	1.9410269	-2.5868977
H	-2.3074180	3.0997356	-2.1322165
O	-0.0203737	1.8225033	0.1107176
H	0.7814507	1.9600018	-0.4253077
H	-0.7479731	2.0179594	-0.5137263
O	3.4670158	-2.5884829	-0.5064943
H	2.8052233	-2.0033561	-0.9358337
H	4.1575910	-2.7238236	-1.1568144
O	-1.2785412	-1.7098882	3.1696492
H	-1.3545067	-1.5850553	4.1169272
H	-1.9977745	-1.1592836	2.7712744
O	-2.9338649	-0.2144429	-0.8739891
H	-2.2186544	-0.6751313	-1.3460605
H	-2.8676967	0.6830254	-1.2300343
H	0.6072589	1.5162738	-3.2774842
O	-0.2571116	1.2090251	-3.5831844
H	-0.2921931	0.2889033	-3.2537267

Table 42: Optimized Cartesian coordinates (in Angstrom) of the gw10-bb-29 structure, which corresponds to the Gly•$(H_2O)_{10}$ cluster after breaking the water bridge.

40
Energy=-1047.3844504960

O	1.8635362	1.6811476	-1.9494180
H	2.7728368	1.9803382	-2.0096195
H	1.9070137	0.7091756	-1.7781420
O	-2.8638296	-0.1019910	1.9086471
H	-2.9397146	-0.2436719	0.9439000
H	-2.5036962	0.7918626	2.0182780
C	0.4236723	-1.2604915	-1.1338683
O	1.6231816	-0.8655083	-1.2782426
O	-0.4755781	-1.2670643	-1.9963097
H	0.1735256	0.2215776	0.9138321
C	0.0672052	-1.7417201	0.2738221
N	0.4645086	-0.7040737	1.2613714
H	-0.0071980	-0.9066483	2.1640886
H	1.4890514	-0.6976564	1.4087527
H	0.6095167	-2.6555089	0.5061268
H	-0.9978619	-1.9146482	0.3739763
O	-1.3693003	2.2559153	2.3781097
H	-1.6597579	3.1393188	2.6098966
H	-0.8418565	2.3582413	1.5675761
O	3.2174254	-0.8280940	1.7977585
H	3.5404359	-1.2077705	2.6168111
H	3.5738127	-1.4005969	1.0875152
O	-2.0823365	2.0034202	-1.9774459
H	-1.4976596	1.6614523	-2.7057733
H	-2.5147014	2.7849185	-2.3264526
O	-0.1401140	1.8212595	-0.0178424
H	0.6491191	1.9720897	-0.5688204
H	-0.8812257	1.9251769	-0.6482875
O	3.6257381	-2.3855367	-0.3483877
H	2.9264773	-1.8767218	-0.8141043
H	4.3205729	-2.5258344	-0.9930974
O	-1.1518419	-1.5671676	3.2896482
H	-1.2338959	-1.3863227	4.2273221
H	-1.9071608	-1.0929489	2.8610935
O	-2.9164194	-0.4655160	-0.8324103
H	-2.1742578	-0.9107173	-1.2768887
H	-2.9104578	0.4071337	-1.2508136
H	0.4937192	1.3186517	-3.3810740
O	-0.3495946	0.9347368	-3.6575010
H	-0.3228905	0.0397929	-3.2640268

Table 43: Optimized Cartesian coordinates (in Angstrom) of the gw10-bb-2 structure, which corresponds to the Gly•$(H_2O)_{10}$ cluster after breaking the water bridge.

40
Energy=-1047.3777804228

O	2.4777489	1.9166658	-1.2804426
H	3.3077730	2.3909712	-1.3605393
H	2.7143853	0.9648045	-1.1643545
O	-1.9678056	0.6041067	2.8170359
H	-2.1478651	0.7562048	1.8781172
H	-1.4267509	1.3684669	3.0826432
C	1.5048077	-1.2074581	-0.8341333
O	2.5957798	-0.6285517	-0.6233925
O	0.9206484	-1.3869023	-1.9368928
H	1.1701078	-0.0182264	1.4452378
C	0.7941052	-1.7505048	0.4101384
N	1.3153106	-1.0367737	1.6012931
H	0.8040711	-1.3272415	2.4567977
H	2.3185947	-1.1819554	1.6636116
H	0.9626542	-2.8187577	0.5137135
H	-0.2771090	-1.5877928	0.3607861
O	-0.0736955	2.5917930	3.2953566
H	-0.2215883	3.5361317	3.3665949
H	0.3282830	2.4547658	2.4196771
O	-1.7630420	0.9704345	-0.0444449
H	-1.7935835	0.0843858	-0.4716871
H	-2.0413624	1.5269204	-0.7880514
O	-2.0041782	1.4197996	-2.8069817
H	-1.0449444	1.3629841	-3.0301195
H	-2.4080879	1.8881131	-3.5394671
O	-0.3188467	-4.0365173	-1.5198686
H	0.1979012	-3.3269068	-1.9209235
H	-1.2117235	-3.6818244	-1.5484619
O	0.7138887	1.5871463	0.8568942
H	-0.1591241	1.4337842	0.4289004
H	1.3237518	1.8630677	0.1470965
O	-0.5872043	-1.5950267	3.4247842
H	-0.7817370	-1.9004227	4.3114405
H	-1.1773806	-0.8199413	3.2625319
O	-1.7902298	-1.2307574	-1.6458677
H	-0.8337070	-1.3216809	-1.8409381
H	-2.1071211	-0.6148440	-2.3212977
H	1.2458321	1.5720702	-2.7760162
O	0.6138298	1.0442369	-3.2837294
H	0.8276139	0.1352329	-3.0050407

Table 44: Optimized Cartesian coordinates (in Angstrom) of the gw10-bb-30 structure, which corresponds to the Gly•$(H_2O)_{10}$ cluster after breaking the water bridge.

40
Energy=-1047.3815952015

O	2.0475840	1.7496536	-2.4454895
H	2.9174306	2.0751841	-2.6854587
H	2.1360232	0.7700411	-2.3706852
O	-2.0266497	-0.7145329	1.8630379
H	-2.2641072	-0.7671851	0.9097527
H	-1.3555063	-0.0066249	1.9193035
C	0.8254499	-1.2844192	-1.6104979
O	1.9816931	-0.8414577	-1.8845053
O	-0.1869032	-1.2516046	-2.3391847
H	0.9344322	-0.0515596	0.6399680
C	0.6625713	-1.9144520	-0.2228972
N	1.2410146	-1.0212517	0.8161174
H	0.9144141	-1.3376927	1.7467607
H	2.2706759	-1.0528511	0.7609126
H	1.1866169	-2.8661845	-0.1787137
H	-0.3833758	-2.0712659	0.0104140
O	-0.1915731	1.2134293	2.5378460
H	-0.8924413	1.6614635	3.0323653
H	0.0507296	1.7868560	1.7983818
O	-2.7279161	1.2904935	3.7314539
H	-2.8696720	0.5326951	3.1436088
H	-3.5871236	1.7033875	3.8263932
O	-1.8307074	1.9181058	-1.6123927
H	-1.3855714	1.6915741	-2.4738204
H	-2.3286342	2.7216125	-1.7746040
O	0.4877431	1.6175516	-0.1004861
H	1.1440086	1.8509823	-0.7794762
H	-0.3650360	1.7688131	-0.5527059
O	3.8741887	-1.1679768	-0.0412705
H	3.3466541	-1.1222679	-0.8700871
H	4.5010485	-1.8835321	-0.1585841
O	-0.0632727	-2.2812100	2.9086276
H	0.0015616	-2.1050988	3.8496772
H	-0.9145423	-1.8793817	2.6366620
O	-2.4912117	-0.7197717	-0.8183894
H	-1.7934737	-1.0716913	-1.4003257
H	-2.5211617	0.2138024	-1.0773409
H	0.4268661	1.5160238	-3.5682332
O	-0.4490892	1.1316114	-3.7144948
H	-0.3227375	0.1987317	-3.4516395

Table 45: Optimized Cartesian coordinates (in Angstrom) of the gw10-bb-31 structure, which corresponds to the Gly•$(H_2O)_{10}$ cluster after breaking the water bridge.

40
Energy=-1047.3807919575

O	2.7240326	1.1658726	-2.6375931
H	3.6401025	1.3397919	-2.8626288
H	2.6433454	0.1815792	-2.5492161
O	-1.7775639	-0.3791299	1.3695806
H	-2.0170942	-0.4564389	0.4187598
H	-1.3165887	0.4713805	1.4513964
C	0.9713213	-1.6288453	-1.9216749
O	2.1838041	-1.3274703	-2.0811703
O	0.0243525	-1.5400267	-2.7364313
H	1.2395275	-0.3295125	0.2390290
C	0.6362457	-2.1376244	-0.5155224
N	1.4222321	-1.3246945	0.4476669
H	1.1353989	-1.5390022	1.4394680
H	2.4097731	-1.4794364	0.2628126
H	0.9238581	-3.1799903	-0.4054940
H	-0.4129132	-2.0197327	-0.2757484
O	-0.1529055	1.9261444	1.9147066
H	-0.5000903	2.8159150	2.0102358
H	0.4127543	1.9481392	1.1198608
O	-2.7774967	0.0917642	3.9237115
H	-2.7016459	-0.1737941	2.9920895
H	-3.4133729	-0.5128441	4.3093249
O	-1.0815385	1.8934638	-2.2031354
H	-0.6214883	1.5411524	-3.0181293
H	-1.4280585	2.7542168	-2.4465563
O	0.9947528	1.3775555	-0.4776826
H	1.7423959	1.4857256	-1.0959399
H	0.2161739	1.5889545	-1.0366574
O	0.0031624	0.3326875	4.3944558
H	-0.9655456	0.2762310	4.4552303
H	0.1342247	1.0015417	3.7105466
O	0.2082008	-1.8500049	2.7612474
H	0.2828659	-1.1796287	3.4743901
H	-0.6289115	-1.5859257	2.3434644
O	-2.2033964	-0.5514212	-1.3199798
H	-1.5626353	-1.0471739	-1.8637652
H	-2.0916720	0.3528587	-1.6490161
H	1.1912870	1.0439199	-3.9398708
O	0.2801799	0.7941138	-4.1473742
H	0.2329260	-0.1403115	-3.8543907

Table 46: Optimized Cartesian coordinates (in Angstrom) of the gw10-bb-32 structure, which corresponds to the Gly•$(H_2O)_{10}$ cluster after breaking the water bridge.

40
Energy=-1047.3831051181

O	3.1573196	0.8311233	-2.3429524
H	4.1122017	0.7972633	-2.2634846
H	2.8228966	-0.0224148	-1.9685097
O	-2.2652827	-0.2529228	4.0145623
H	-3.2029415	-0.2281161	4.2153236
H	-2.1042973	0.5407833	3.4507023
C	0.8278162	-1.5895907	-1.5602155
O	2.0053381	-1.2770068	-1.2381771
O	0.2701548	-1.5237323	-2.6778579
H	0.1627862	-0.4584755	0.7661904
C	-0.0200910	-2.1191832	-0.3930231
N	0.4670584	-1.4542099	0.8367994
H	0.1122234	-1.8777303	1.7192541
H	1.4865820	-1.4594481	0.7656372
H	0.1126336	-3.1938621	-0.2974503
H	-1.0723554	-1.8940404	-0.5291726
O	-1.8225550	1.8290567	2.4050029
H	-1.4174296	2.6460627	2.6995474
H	-1.3815553	1.6119603	1.5542656
O	0.0094048	-1.1033575	5.4648094
H	-0.8185444	-0.6571422	5.2295842
H	-0.0166664	-1.2062938	6.4171035
O	-0.4402029	2.2534389	-3.5439557
H	0.1776165	1.5954045	-3.9624056
H	-0.7001306	2.8524066	-4.2462969
O	1.1712719	2.5090911	-1.2125416
H	1.9591800	2.0339331	-1.5259846
H	0.6455955	2.6368935	-2.0193077
O	-0.5432802	0.9996341	0.1718464
H	-1.1069439	0.7440298	-0.6019295
H	0.1424167	1.5791606	-0.2504273
O	-0.7020187	-2.4340652	3.1154207
H	-0.2131746	-2.3217001	3.9453511
H	-1.4454204	-1.8267836	3.2626841
O	-1.8144273	0.2601420	-2.0778959
H	-1.2491734	-0.4587769	-2.4139803
H	-1.5794534	1.0064155	-2.6542578
H	2.0771269	0.6219289	-3.9492508
O	1.2441447	0.4054175	-4.3933747
H	0.9521763	-0.3952934	-3.9116332

Table 47: Optimized Cartesian coordinates (in Angstrom) of the gw10-bb-33 structure, which corresponds to the Gly•$(H_2O)_{10}$ cluster after breaking the water bridge.

40
Energy=-1047.3815952610

O	2.3737992	1.4051888	-2.3720768
H	3.2891155	1.6123038	-2.5708121
H	2.3342656	0.4250551	-2.2682693
O	-2.1937356	-0.3986422	1.7667574
H	-2.3874077	-0.4519652	0.8036519
H	-1.4427408	0.2219517	1.8411407
C	0.7379466	-1.4266491	-1.5309516
O	1.9529916	-1.1390586	-1.7525249
O	-0.2238165	-1.2923778	-2.3144793
H	0.8871400	-0.1461653	0.6905683
C	0.4268711	-1.9870906	-0.1387967
N	1.0597421	-1.1403935	0.9073544
H	0.6490209	-1.3839568	1.8265269
H	2.0786561	-1.3016684	0.9090595
H	0.8239821	-2.9947601	-0.0424511
H	-0.6409757	-2.0050469	0.0412009
O	-0.1668216	1.3060105	2.4925443
H	-0.8300315	1.8522490	2.9378816
H	0.1825803	1.8224000	1.7538896
O	-2.7299659	1.7339806	3.5466432
H	-2.9363319	0.9826367	2.9697804
H	-3.5330696	2.2549541	3.5834151
O	-1.4903204	2.0778283	-1.7580528
H	-1.0335375	1.7705602	-2.5878016
H	-1.8750942	2.9309618	-1.9677806
O	0.6915102	1.5416796	-0.1138449
H	1.4058045	1.6705518	-0.7614377
H	-0.1111864	1.7830704	-0.6158440
O	3.6936230	-1.6419403	0.1981144
H	4.2289308	-2.4343318	0.1324532
H	3.2190557	-1.5558988	-0.6589708
O	-0.4969781	-2.1612192	2.9573800
H	-0.4578912	-1.9626367	3.8953741
H	-1.2763408	-1.6663967	2.6289749
O	-2.5174491	-0.4306660	-0.9350680
H	-1.8411977	-0.8849871	-1.4694936
H	-2.4154518	0.4909551	-1.2174460
H	0.7962879	1.3364939	-3.5773922
O	-0.1126454	1.0598136	-3.7609348
H	-0.1183338	0.1272062	-3.4682824

Table 48: Optimized Cartesian coordinates (in Angstrom) of the gw10-bb-3 structure, which corresponds to the Gly•$(H_2O)_{10}$ cluster after breaking the water bridge.

40
Energy=-1047.3799685944

O	3.6268084	0.1252823	-2.8832192
H	3.4810537	-0.6969283	-3.3751439
H	3.3192154	-0.1313798	-1.9983317
O	-2.1278705	-0.2728066	3.3861125
H	-2.5231603	-0.2031107	2.5054732
H	-1.7679330	0.6117018	3.5687791
C	1.0102535	-1.1493404	-0.7519593
O	2.1690787	-0.7137768	-0.5900375
O	0.4093727	-1.4144078	-1.8335932
H	0.4231340	0.3610085	1.5430916
C	0.2302224	-1.4155375	0.5421601
N	0.8419516	-0.5806872	1.6020307
H	0.7067189	-0.9951269	2.5405126
H	1.8280982	-0.5033852	1.3210293
H	0.3336752	-2.4620804	0.8168171
H	-0.8210892	-1.1730011	0.4476384
O	-0.7079499	2.1270446	3.6365870
H	-0.8849580	2.9606463	4.0752660
H	-0.6006676	2.3378563	2.6941583
O	-2.9977182	0.3530242	0.7075107
H	-2.7267194	0.0898770	-0.2116256
H	-3.9196131	0.6110015	0.6385823
O	-0.4293374	2.3293145	-1.7218216
H	0.2408004	1.8918259	-2.3255298
H	-0.6070353	3.1851805	-2.1172184
O	2.3717072	-2.3272316	-3.7011863
H	1.9264022	-2.5142422	-4.5294083
H	1.6523228	-2.1066386	-3.0847732
O	-0.6093662	1.7618012	0.9444610
H	-1.5230593	1.4292416	0.8741086
H	-0.4103959	2.0825805	0.0400028
O	-0.0738873	-1.9468875	3.7716361
H	0.1233803	-2.0960965	4.6974963
H	-0.9138361	-1.4364098	3.7499559
O	-2.0282379	-0.0727824	-1.7033245
H	-1.2867433	-0.6982597	-1.8190117
H	-1.6248766	0.7916656	-1.8812117
H	2.0378241	0.8654341	-3.2573574
O	1.0603007	0.9372879	-3.3167112
H	0.7921341	0.0583424	-3.0019450

Table 49: Optimized Cartesian coordinates (in Angstrom) of the gw10-bb-4 structure, which corresponds to the Gly•$(H_2O)_{10}$ cluster after breaking the water bridge.

40
Energy=-1047.3847635745

O	3.8799113	0.7922989	-2.5695870
H	4.5740036	0.2797528	-2.9875140
H	3.5287084	0.2074399	-1.8665578
O	-1.7448369	0.1910062	3.5055724
H	-2.2518986	0.2492647	2.6816212
H	-1.2066443	0.9994086	3.5218600
C	1.5159810	-1.2833948	-0.9128292
O	2.5780772	-0.6638894	-0.6600691
O	1.1155507	-1.7251824	-2.0183848
H	0.5569406	0.3027554	1.2386769
C	0.6040614	-1.5261262	0.3000475
N	1.0365187	-0.6034063	1.3744306
H	0.8480475	-0.9834701	2.3189374
H	2.0344741	-0.4451812	1.1844295
H	0.7105504	-2.5512264	0.6446070
H	-0.4371326	-1.3434930	0.0570006
O	0.1198322	2.2862951	3.2183164
H	0.2026817	3.1616259	3.5998529
H	0.0592571	2.4184809	2.2575879
O	-2.9140289	0.7084587	0.9486315
H	-2.8361567	0.2823838	0.0516588
H	-3.7733040	1.1354025	0.9526981
O	-0.4410929	1.7586374	-2.1261195
H	0.2722728	1.3363744	-2.6929406
H	-0.6962529	2.5514608	-2.6031314
O	-1.4151173	-2.5824311	-2.0495677
H	-1.6088240	-3.0946532	-2.8362334
H	-0.4561914	-2.3588200	-2.1076923
O	-0.3709485	1.7168005	0.6141620
H	-1.3206674	1.5174947	0.7229611
H	-0.2621685	1.8466043	-0.3507790
O	0.0599153	-1.7709486	3.6460614
H	0.3467875	-1.9348299	4.5455785
H	-0.6854856	-1.1302532	3.7116671
O	-2.4780743	-0.1387366	-1.4814334
H	-2.1888573	-1.0357795	-1.7456039
H	-1.8157482	0.4672467	-1.8514889
H	2.2540890	0.7830461	-3.4051178
O	1.3280823	0.5418039	-3.5970806
H	1.2776878	-0.3622203	-3.2342285

Table 50: Optimized Cartesian coordinates (in Angstrom) of the gw10-bb-5 structure, which corresponds to the Gly•$(H_2O)_{10}$ cluster after breaking the water bridge.

40
Energy=-1047.3766450629

O	3.6619572	0.4904791	-3.0402122
H	4.1553907	-0.1379949	-3.5698484
H	3.1620413	-0.0609428	-2.4020275
O	-2.0673053	-0.1406376	2.9207326
H	-2.4443177	-0.0245997	2.0353876
H	-1.6171979	0.7017693	3.1070601
C	0.8347202	-1.0788641	-1.4240874
O	2.0536294	-0.8132198	-1.2738141
O	0.1558081	-1.0909886	-2.4795080
H	0.5886873	0.1971342	0.9897304
C	0.1046627	-1.4465189	-0.1245996
N	0.8516327	-0.8000972	0.9817900
H	0.6796822	-1.2281957	1.8996401
H	1.8345654	-0.8668279	0.6922790
H	0.1429021	-2.5206842	0.0270299
H	-0.9214800	-1.0986049	-0.1194562
O	-0.3899884	2.0700405	3.2115240
H	-0.4974227	2.9254502	3.6304111
H	-0.2414445	2.2539226	2.2674620
O	-2.8800353	0.6712482	0.3158019
H	-2.6840845	0.4668659	-0.6425065
H	-3.7552669	1.0651651	0.3171791
O	-0.2184874	2.5176743	-2.1110864
H	0.3653815	2.0446749	-2.7782399
H	-0.2639845	3.4260588	-2.4161991
O	1.2730857	-3.6578321	1.8361240
H	1.3372627	-4.6129690	1.8767755
H	0.6703663	-3.4071920	2.5482634
O	-0.3170296	1.7529615	0.5135701
H	-1.2640364	1.5263865	0.4623862
H	-0.1211380	2.1136184	-0.3772121
O	-0.1433970	-1.8915004	3.4481401
H	0.1600022	-1.6725657	4.3317688
H	-0.9474294	-1.3344575	3.3071531
O	-2.1276771	0.3632702	-2.1623448
H	-1.4325912	-0.3073569	-2.3343320
H	-1.6552588	1.1975027	-2.3100779
H	2.0645104	1.0539555	-3.7250913
O	1.0999036	1.1191825	-3.8550251
H	0.7933813	0.2346895	-3.5745407

Table 51: Optimized Cartesian coordinates (in Angstrom) of the gw10-bb-6 structure, which corresponds to the Gly•$(H_2O)_{10}$ cluster after breaking the water bridge.

40
Energy=-1047.3869504639

O	2.3202830	1.5357026	-1.5025760
H	3.1986146	1.9111809	-1.5897557
H	2.4458299	0.5595404	-1.4179622
O	-2.3037078	0.7714521	2.6280055
H	-2.4187863	0.9584345	1.6839921
H	-1.6249998	1.4078450	2.9131329
C	1.0322974	-1.4643383	-1.0905648
O	2.2161608	-1.0446000	-0.9254036
O	0.3688798	-1.4543102	-2.1479288
H	0.8319692	-0.3576177	1.2229602
C	0.3356630	-2.0422822	0.1468743
N	0.8182274	-1.3815119	1.3857181
H	0.1616318	-1.5778902	2.1651874
H	1.7741710	-1.6925149	1.6005572
H	0.5429949	-3.1076000	0.2185042
H	-0.7381338	-1.9008995	0.0801798
O	-0.0639540	2.3670051	3.1435103
H	-0.0628364	3.3219439	3.2258098
H	0.3097529	2.1816632	2.2634097
O	-1.9641926	1.0907101	-0.1956906
H	-2.1069515	0.2113798	-0.6196360
H	-2.1787045	1.6746022	-0.9401411
O	-2.2167995	1.6324441	-2.9264557
H	-1.2784259	1.4706402	-3.1833441
H	-2.5828586	2.1725146	-3.6285886
O	3.3726085	-2.3991432	1.0962695
H	3.2154277	-1.9216538	0.2557837
H	4.3029852	-2.2955106	1.2999347
O	0.5749327	1.3350123	0.6741725
H	-0.3192046	1.3108700	0.2602559
H	1.1989660	1.5676929	-0.0370504
O	-1.3223119	-1.6686446	3.0343962
H	-1.5660054	-1.9930096	3.9020851
H	-1.7608176	-0.7870340	2.9394092
O	-2.3177723	-1.0751732	-1.7687903
H	-1.4057950	-1.3352253	-2.0083965
H	-2.5624052	-0.4371077	-2.4516674
H	1.0205106	1.4215520	-2.9890247
O	0.3280242	0.9806722	-3.5001744
H	0.4247322	0.0532088	-3.2169974

Table 52: Optimized Cartesian coordinates (in Angstrom) of the gw10-bb-7 structure, which corresponds to the Gly•$(H_2O)_{10}$ cluster after breaking the water bridge.

40
Energy=-1047.3838662927

O	2.4470815	1.3702954	-1.7735839
H	3.3367539	1.7198705	-1.8538822
H	2.5421069	0.3853504	-1.7193187
O	-1.8932633	0.5778041	2.4777333
H	-2.0538440	0.7776171	1.5411084
H	-1.2234272	1.2225950	2.7525162
C	1.0814208	-1.6052220	-1.4386822
O	2.2517785	-1.1871739	-1.2598775
O	0.3979380	-1.6031618	-2.4904355
H	0.9822534	-0.5366426	0.9135911
C	0.4031756	-2.1824552	-0.1893808
N	1.0077779	-1.5698722	1.0145349
H	0.4964502	-1.8172650	1.8722027
H	1.9912486	-1.8110464	1.0935159
H	0.5413176	-3.2603092	-0.1516934
H	-0.6603545	-1.9663132	-0.1824503
O	0.4954297	2.0694809	2.9404621
H	0.6617793	2.9948119	3.1295703
H	0.7089330	1.9390639	1.9928880
O	-1.8051787	0.9450543	-0.3343183
H	-1.9641934	0.0856200	-0.7953990
H	-2.0517922	1.5627911	-1.0416603
O	-2.1455900	1.6042904	-3.0077931
H	-1.2195570	1.4208558	-3.2966449
H	-2.5097806	2.1842609	-3.6783488
O	1.7045412	-0.4784518	3.5957962
H	0.9177516	-0.9156601	3.9379694
H	1.4501688	0.4539020	3.5770109
O	0.7645648	1.1769400	0.4188264
H	-0.1393041	1.1708909	0.0270814
H	1.3831022	1.3888291	-0.3075251
O	-0.8561152	-1.7929084	3.1093712
H	-1.5221427	-2.4190945	3.3982598
H	-1.3417871	-0.9584375	2.8953014
O	-2.2269798	-1.1622893	-1.9534283
H	-1.3316094	-1.4309359	-2.2533905
H	-2.5098517	-0.5176492	-2.6144651
H	1.0882797	1.3075273	-3.2085215
O	0.3532822	0.8996586	-3.6867436
H	0.4476353	-0.0426210	-3.4501967

Table 53: Optimized Cartesian coordinates (in Angstrom) of the gw10-bb-8 structure, which corresponds to the Gly•$(H_2O)_{10}$ cluster after breaking the water bridge.

40
Energy=-1047.3905019654

O	3.1220319	0.4753920	-1.5465542
H	4.0707607	0.5075768	-1.6850718
H	2.8853089	-0.4812077	-1.4884737
O	-1.1957540	-0.0516344	2.7914617
H	-1.8536932	0.0489097	2.0861078
H	-0.7847035	0.8272608	2.8917414
C	0.8109718	-1.8531994	-1.1418754
O	2.0679877	-1.9018147	-1.0940019
O	0.0788905	-1.6470316	-2.1369079
H	1.2282531	-0.7393756	1.2654364
C	0.1018023	-2.0737207	0.2013495
N	1.0725972	-1.7688371	1.2768083
H	0.7532003	-2.0886380	2.2063436
H	1.9557255	-2.1890521	0.9834847
H	-0.2211978	-3.1077939	0.2917228
H	-0.7561942	-1.4199246	0.3095692
O	0.1447619	2.4065207	2.7789150
H	0.9545645	2.0620235	2.3805054
H	-0.2734558	2.8360251	2.0223524
O	-2.8460296	0.3815246	0.5546890
H	-2.7131358	0.0136787	-0.3635374
H	-3.7925676	0.5028707	0.6532086
O	-1.0279713	2.0307805	-2.7551366
H	-0.2223220	1.5471620	-3.0819847
H	-1.2516379	2.6593259	-3.4440453
O	1.4957738	0.9037681	0.7267683
H	0.6916439	1.3394857	0.3683426
H	2.1454536	0.9178356	0.0022555
O	-0.7874500	2.2228322	0.0076635
H	-1.5825029	1.7074465	0.2255544
H	-0.8545345	2.3550022	-0.9554302
O	-0.2731658	-2.4082979	3.5829207
H	-0.1418497	-2.5440691	4.5221066
H	-0.7249098	-1.5417710	3.4880827
O	-2.3186893	-0.3752463	-1.8889198
H	-1.5316996	-0.9516595	-1.9896675
H	-2.0487181	0.4488643	-2.3236384
H	1.8384576	0.7189297	-3.0042621
O	1.0253620	0.5616326	-3.5058219
H	0.7586351	-0.3315743	-3.2120614

Table 54: Optimized Cartesian coordinates (in Angstrom) of the gw10-bb-9 structure, which corresponds to the Gly•$(H_2O)_{10}$ cluster after breaking the water bridge.

40
Energy=-1047.3833358281

O	3.4115610	0.1145003	-3.1780243
H	3.8084023	-0.5644131	-3.7267214
H	2.9245211	-0.3787925	-2.4857620
O	-2.3328492	0.1307877	3.2398311
H	-2.6928187	0.2481097	2.3481307
H	-1.7002178	0.8612863	3.3462677
C	0.7065321	-1.3474600	-1.2449558
O	1.9338793	-1.0565021	-1.2017980
O	-0.0419848	-1.3396689	-2.2479866
H	0.4142862	-0.0375792	1.0955502
C	0.0670090	-1.7836132	0.0778324
N	0.6322298	-1.0364589	1.2271662
H	0.1998581	-1.3795183	2.1075005
H	1.6560804	-1.1628765	1.2775727
H	0.2561387	-2.8434615	0.2337890
H	-1.0052766	-1.6193069	0.0586964
O	-0.2337979	2.0009657	3.2355054
H	-0.1542040	2.8737253	3.6235247
H	-0.1432178	2.1276706	2.2754340
O	-3.0483724	0.7456652	0.5412988
H	-2.8807661	0.4038948	-0.3779672
H	-3.8718070	1.2350260	0.4817512
O	-0.4175320	2.2573654	-2.0975999
H	0.1248532	1.7611269	-2.7787251
H	-0.4780480	3.1562712	-2.4269192
O	3.3416450	-1.6872003	0.9842096
H	4.1436912	-1.1817752	1.1281390
H	3.0639799	-1.4892089	0.0653974
O	-0.3835293	1.5515773	0.5542564
H	-1.3492104	1.4157624	0.5696817
H	-0.2169619	1.8774113	-0.3540704
O	-0.8413245	-2.0697602	3.2920843
H	-0.6255941	-2.3549526	4.1812255
H	-1.4727231	-1.3182956	3.3909510
O	-2.3437521	0.1275425	-1.9107723
H	-1.6666908	-0.5605457	-2.0633217
H	-1.8652368	0.9419240	-2.1318783
H	1.7678700	0.7078299	-3.7868319
O	0.7974081	0.7654416	-3.8474274
H	0.5159699	-0.0924943	-3.4750344

Table 55: Optimized Cartesian coordinates (in Angstrom) of the gw9-bb-10 structure, which corresponds to the Gly•$(H_2O)_9$ cluster after breaking the water bridge.

37
Energy=-971.0372011066

O	0.0136653	1.7675229	-3.8647663
H	-0.4352472	2.4784672	-4.3226908
H	-0.4503728	1.6586380	-3.0117048
O	0.0504482	-1.8459243	3.3680212
H	0.8111265	-1.2553965	3.2622755
H	-0.5689199	-1.2363837	3.8228173
C	0.9715871	0.8514476	1.5708575
O	0.0457739	1.5620977	1.0744795
O	1.2391238	0.6703921	2.7722607
H	0.3766408	0.1240316	-0.9180599
C	1.8667180	0.1370079	0.5441449
N	1.0467826	-0.5396646	-0.4920890
H	1.6410122	-0.9365756	-1.2445761
H	0.4759043	-1.2852113	-0.0573399
H	2.4885961	-0.6053507	1.0333672
H	2.4999866	0.8692446	0.0480365
O	-2.7047442	-0.3073072	-0.0071709
H	-2.8203264	0.2952251	0.7462617
H	-2.1727261	-1.0318295	0.3534563
O	-0.7005730	-2.2307612	0.9008992
H	-0.4628261	-2.1288911	1.8697731
H	-0.8565572	-3.1696677	0.7747286
O	2.5095965	-1.5102455	-2.6194282
H	2.1078751	-1.1492611	-3.4425625
H	3.4557413	-1.5043635	-2.7718897
O	-0.9734218	1.2444427	-1.4025637
H	-1.7091700	0.6861606	-1.0609305
H	-0.6360323	1.6557949	-0.5819667
O	-2.4173714	1.5898980	2.0914875
H	-1.4820928	1.7209014	1.8034275
H	-2.8031855	2.4673845	2.1322970
O	-1.1189916	0.4051595	4.3674906
H	-1.7916978	0.7840056	3.7845681
H	-0.2987811	0.7779581	4.0038149
O	1.3051738	-0.4313466	-4.7564969
H	0.6808111	-0.9605509	-5.2550685
H	0.8164740	0.3829510	-4.5151604

Table 56: Optimized Cartesian coordinates (in Angstrom) of the gw9-bb-11 structure, which corresponds to the Gly•$(H_2O)_9$ cluster after breaking the water bridge.

37
Energy=-971.0369115795

O	-0.2278427	2.0784656	-3.0549896
H	-0.7246615	2.7963134	-3.4514063
H	-0.6879495	1.8498013	-2.2130051
O	-1.0327977	-1.6408614	3.6240805
H	-0.3083387	-1.0082049	3.7970829
H	-1.7994283	-1.0521528	3.5342996
C	0.6968303	0.6055307	2.2401513
O	-0.3542770	1.1600811	1.7781290
O	0.9259471	0.2759494	3.4132140
H	0.4121372	0.1926537	-0.3813141
C	1.7686696	0.2822350	1.1901980
N	1.1252481	-0.4183069	0.0454152
H	1.7933047	-0.6685824	-0.6923401
H	0.6291891	-1.2588228	0.3830760
H	2.5218120	-0.3705046	1.6176499
H	2.2208938	1.1883722	0.7978717
O	-2.7907734	-0.7953338	0.1572359
H	-3.0188717	-0.3805184	1.0055537
H	-2.1609040	-1.4839993	0.4163274
O	-0.5646211	-2.3947051	1.1629158
H	-0.7292291	-2.1594464	2.1245881
H	-0.4974674	-3.3521787	1.1485845
O	2.5580162	-0.9285463	-2.3868054
H	1.8336641	-0.8388700	-3.0444301
H	3.2110741	-1.5050802	-2.7869622
O	-1.1477096	1.1601326	-0.7627530
H	-1.8353829	0.4798506	-0.5834790
H	-0.8892917	1.4341469	0.1453082
O	-2.7058246	0.4359260	2.7187581
H	-1.8296219	0.8447211	2.4936938
H	-3.1927876	1.1029768	3.2061646
O	2.2543411	1.8588955	-1.5588733
H	1.5510251	2.1705983	-2.1426220
H	2.6552222	1.1322965	-2.0476720
O	0.4838514	-0.3834057	-4.0174668
H	-0.3067882	-0.9214213	-4.0858973
H	0.1633423	0.5119941	-3.7902821

Table 57: Optimized Cartesian coordinates (in Angstrom) of the gw9-bb-12 structure, which corresponds to the Gly•$(H_2O)_9$ cluster after breaking the water bridge.

37
Energy=-971.0362132498

O	-0.5858576	1.7926476	-2.1328665
H	-1.4839427	1.4931195	-1.9491461
H	-0.2600323	2.0503046	-1.2509808
O	-1.3300851	-0.9750909	2.3968215
H	-0.3967454	-0.7532948	2.2479549
H	-1.7353430	-0.0944955	2.2966295
C	1.0609332	1.0360108	0.7636036
O	0.3056943	2.0065708	0.5271578
O	1.1178042	0.3189044	1.8002297
H	1.2199458	-1.2020671	-0.5616511
C	2.0505710	0.6574197	-0.3392647
N	2.1700698	-0.8215769	-0.3559002
H	2.8171512	-1.1210986	-1.1017168
H	2.4372159	-1.1291215	0.5763386
H	3.0265250	1.0868716	-0.1282692
H	1.7150173	0.9783392	-1.3168108
O	-2.5738528	0.3054091	-0.5234437
H	-2.6138835	0.8116356	0.3042960
H	-3.0248753	-0.5229903	-0.3194479
O	-2.4016913	-2.4742582	0.4841007
H	-2.0305215	-2.0091123	1.2743117
H	-2.8262613	-3.2672664	0.8149383
O	3.2717421	-0.9468529	-2.8191200
H	2.4067809	-0.6810041	-3.2051071
H	3.7580958	-1.3818786	-3.5202618
O	-0.1606835	1.7221863	3.9999569
H	0.3589876	1.2784219	3.3078527
H	-0.1527678	1.1001369	4.7297772
O	-2.0323468	1.7202467	1.8660324
H	-1.1819450	1.9424243	1.4256009
H	-1.8300572	1.9368414	2.7874583
O	-0.4183938	-1.4115928	-1.0445616
H	-0.9759043	-2.0960263	-0.6310386
H	-0.9790158	-0.6215258	-0.9103269
O	0.7295768	-0.3068780	-3.4303729
H	0.2246562	-0.9542140	-2.9209676
H	0.3234391	0.5328544	-3.1418063

Table 58: Optimized Cartesian coordinates (in Angstrom) of the gw9-bb-13 structure, which corresponds to the Gly•$(H_2O)_9$ cluster after breaking the water bridge.

37
Energy=-971.0465842139

O	-1.1424792	0.9629775	-1.3981548
H	-2.0871731	0.7944189	-1.1760691
H	-0.8308619	1.4955011	-0.6404724
O	-2.0348460	-0.6272147	3.0653420
H	-1.1096510	-0.3149323	2.9925874
H	-2.5333327	0.1935201	2.9357738
C	0.4941089	0.9942981	1.4201650
O	-0.3177650	1.8915749	1.0704966
O	0.4713843	0.2620783	2.4357223
H	1.2612660	-1.2156741	0.1312925
C	1.6816521	0.7489142	0.4792196
N	2.0341910	-0.6862290	0.5945257
H	2.9490023	-0.9003748	0.1625720
H	1.9903553	-0.9008704	1.5929434
H	2.5320179	1.3496570	0.7920806
H	1.4491947	0.9739604	-0.5551277
O	-3.5520934	0.3340161	-0.3383073
H	-3.5144947	0.9108862	0.4416031
H	-3.3698051	-0.5476928	0.0201459
O	-2.4471610	-2.0538299	0.8928666
H	-2.2996873	-1.5799446	1.7576067
H	-2.9003225	-2.8689727	1.1166642
O	3.1128386	0.5643589	-2.7871107
H	2.1959371	0.3055448	-3.0287753
H	3.4242877	1.1229971	-3.5001010
O	4.3595847	-0.8394160	-0.8727519
H	4.0330826	-0.3542957	-1.6601765
H	4.8814905	-1.5678503	-1.2124234
O	-2.8383875	1.8503948	1.9697404
H	-1.8846302	1.9636371	1.7347290
H	-3.1269400	2.6996582	2.3087005
O	-0.2189785	-1.5396714	-0.6752645
H	-0.9374544	-1.9199282	-0.1342390
H	-0.5800362	-0.6610121	-0.9202426
O	0.5661227	-0.1656851	-3.2704900
H	0.3732155	-1.0540021	-2.9542865
H	-0.0836322	0.3792024	-2.7907847

Table 59: Optimized Cartesian coordinates (in Angstrom) of the gw9-bb-14 structure, which corresponds to the Gly•$(H_2O)_9$ cluster after breaking the water bridge.

37
Energy=-971.0340092638

O	-0.5055512	1.7223902	-1.4599834
H	-1.4460240	1.5108817	-1.4231926
H	-0.2675730	1.8338989	-0.5142065
O	-1.7171267	-0.9610008	3.1822597
H	-0.7890550	-0.7017103	3.0044446
H	-2.1747650	-0.1103335	3.1304839
C	0.8328321	0.6953730	1.4571240
O	0.0693902	1.6811821	1.2536893
O	0.7717240	-0.1778411	2.3482127
H	1.1180681	-1.2691193	-0.0882642
C	1.9806365	0.5206444	0.4616470
N	2.0766180	-0.9347272	0.1639684
H	2.7109805	-1.0991797	-0.6289376
H	2.3473988	-1.4282258	1.0101122
H	2.9172723	0.8493345	0.9044967
H	1.8316329	1.0543564	-0.4684362
O	-2.6717466	0.1960005	-0.1547465
H	-2.7101286	0.7409072	0.6540938
H	-3.1094686	-0.6266600	0.0974374
O	-2.4964638	-2.4579148	1.1448995
H	-2.2328717	-1.9537354	1.9600327
H	-2.9183110	-3.2587606	1.4601512
O	3.0513512	-0.6696100	-2.4144444
H	2.1159990	-0.6620682	-2.7337014
H	3.5736614	-1.0580483	-3.1186903
O	2.3075603	2.4460125	-2.2828717
H	1.3478913	2.4361311	-2.3617146
H	2.5909434	1.5906939	-2.6188239
O	-2.3816368	1.6189045	2.2056789
H	-1.4200181	1.7357838	1.9874074
H	-2.7013112	2.4816859	2.4756156
O	-0.5301650	-1.5410231	-0.4936319
H	-1.0575430	-2.1735980	0.0309103
H	-1.0995001	-0.7473294	-0.4178862
O	0.4531006	-0.4771362	-2.8965022
H	-0.0057203	-1.1531277	-2.3790700
H	0.1379193	0.3469687	-2.4775616

Table 60: Optimized Cartesian coordinates (in Angstrom) of the gw9-bb-15 structure, which corresponds to the Gly•$(H_2O)_9$ cluster after breaking the water bridge.

37
Energy=-971.0492149638

O	-1.0733274	1.2709725	-1.6378272
H	-2.0122618	1.1478987	-1.3721941
H	-0.6872200	1.7054119	-0.8552028
O	-1.7550147	-0.6660771	2.7866486
H	-0.8206125	-0.4214659	2.6363405
H	-2.1981443	0.1952893	2.7684173
C	0.7802530	0.9143148	1.0602726
O	-0.0292009	1.8570519	0.8739970
O	0.7837441	0.0806019	2.0019157
H	1.2733154	-1.1036333	-0.5013117
C	1.8927022	0.7859523	0.0131789
N	2.1820448	-0.6373786	-0.2905853
H	2.7642195	-0.6832852	-1.1399847
H	2.6356909	-1.0928920	0.5146363
H	2.8001423	1.2535292	0.3890207
H	1.6067440	1.2764827	-0.9104265
O	-3.4480487	0.6985019	-0.4372341
H	-3.3220930	1.1968906	0.3854724
H	-3.3295423	-0.2235845	-0.1638968
O	-2.4997722	-1.8595401	0.5567893
H	-2.2379774	-1.4848938	1.4408073
H	-2.9744993	-2.6711178	0.7457699
O	3.1370318	-0.1581835	-2.8234297
H	2.2471610	-0.0633952	-3.2267744
H	3.7230187	-0.4197774	-3.5347324
O	2.9128264	-1.5358159	2.2208109
H	3.5519657	-1.3495342	2.9100177
H	2.1404072	-0.9579658	2.3977604
O	-2.4818157	1.9351382	1.9597997
H	-1.5432229	1.9945766	1.6611978
H	-2.6767927	2.7743411	2.3807763
O	-0.3392381	-1.3349248	-1.0884644
H	-1.0394325	-1.7176797	-0.5262876
H	-0.6595457	-0.4229760	-1.2527699
O	0.5361207	-0.0413669	-3.5775646
H	0.1825886	-0.8649395	-3.2223851
H	-0.0222142	0.6234736	-3.1425581

Table 61: Optimized Cartesian coordinates (in Angstrom) of the gw9-bb-16 structure, which corresponds to the Gly•$(H_2O)_9$ cluster after breaking the water bridge.

37
Energy=-971.0428655011

O	-1.0182693	1.7798957	-1.6794053
H	-1.8511327	1.3126304	-1.5355788
H	-0.7519373	2.0291293	-0.7740391
O	-2.0152749	-0.7291390	3.0599892
H	-1.1165704	-0.3603708	2.9440249
H	-2.5626106	0.0565915	2.9221365
C	0.4369636	1.1135426	1.3551316
O	-0.3530084	2.0389852	1.0324227
O	0.3993306	0.3605163	2.3556972
H	1.1335584	-1.0967560	0.0640398
C	1.6110893	0.8540710	0.4015636
N	1.9245813	-0.5912478	0.5061306
H	2.8336591	-0.8414601	0.0755164
H	1.8765531	-0.8032879	1.5060081
H	2.4797730	1.4277219	0.7145544
H	1.3711976	1.0906192	-0.6277077
O	-2.8806511	0.0407810	-0.3386723
H	-3.0149504	0.6387352	0.4194898
H	-3.1438788	-0.8286328	-0.0087261
O	-2.4461467	-2.4397949	1.0757324
H	-2.2958758	-1.8631532	1.8700673
H	-2.8559348	-3.2398347	1.4085855
O	3.1990971	0.4162128	-2.8646118
H	2.2363500	0.2337088	-2.9618226
H	3.4814963	0.8052323	-3.6926525
O	4.2949756	-0.9211229	-0.8444289
H	4.7697458	-1.7078982	-1.1165093
H	4.0388612	-0.4621684	-1.6746330
O	-2.8422536	1.7176415	1.8809975
H	-1.8970048	1.9527395	1.6969079
H	-3.2948100	2.5472269	2.0433248
O	-0.4789439	-1.4508168	-0.5868115
H	-0.9858968	-2.1085380	-0.0780487
H	-1.1127385	-0.7090447	-0.5803975
O	0.5732451	-0.0684346	-2.9282752
H	0.2408426	-0.8491254	-2.4704367
H	0.0165692	0.6548453	-2.5695632

Table 62: Optimized Cartesian coordinates (in Angstrom) of the gw9-bb-17 structure, which corresponds to the Gly•$(H_2O)_9$ cluster after breaking the water bridge.

37
Energy=-971.0370131079

O	-0.8354360	1.3881028	-2.1273444
H	-1.0570934	1.9152084	-2.8968767
H	-1.6980841	1.1967365	-1.6825016
O	-1.6379012	-1.3950673	1.9406838
H	-0.7335045	-1.1179271	2.1827076
H	-2.1347014	-0.5586846	1.9799212
C	0.7149841	0.8754737	1.6884830
O	-0.0421024	1.7947900	2.0708180
O	0.8743371	-0.2736073	2.1806620
H	1.4332805	-0.5389857	-0.7010283
C	1.5713031	1.1803951	0.4476606
N	2.1095871	-0.1136766	-0.0360094
H	3.0252293	-0.0680187	-0.5063633
H	2.1098082	-0.7014179	0.8114412
H	2.3920125	1.8363981	0.7235845
H	0.9716756	1.6480453	-0.3266618
O	-3.0563436	0.5549977	-0.9188630
H	-3.1730217	0.8529882	-0.0021933
H	-2.8727950	-0.3928708	-0.8429194
O	-1.8689543	-2.0655509	-0.5764217
H	-1.7507528	-1.8925439	0.4005733
H	-2.2725154	-2.9334195	-0.6409299
O	2.5222890	-1.6885541	-3.3597851
H	1.6377933	-1.5597761	-2.9677217
H	2.3894705	-1.6423482	-4.3077615
O	4.2316831	-0.2055858	-1.8280507
H	5.1182815	-0.5688612	-1.8071252
H	3.7433416	-0.7382346	-2.4874197
O	-2.7299211	1.2262482	1.7717001
H	-1.8144473	1.5587722	1.7121993
H	-2.9161358	1.3752599	2.7099890
O	-1.6414926	1.4973410	4.3672178
H	-1.4013549	0.7219619	4.8778393
H	-0.9176043	1.5875766	3.7208136
O	0.2841459	-1.0350446	-1.9127666
H	-0.4471610	-1.5478962	-1.5102152
H	-0.1278996	-0.1722240	-2.1473356

Table 63: Optimized Cartesian coordinates (in Angstrom) of the gw9-bb-18 structure, which corresponds to the Gly•$(H_2O)_9$ cluster after breaking the water bridge.

37
Energy=-971.0350607400

O	-1.6669416	1.5198992	-1.9973319
H	-1.3400671	1.8762128	-1.1534786
H	-2.3030268	0.8489400	-1.6855817
O	-1.7448532	-0.6529580	3.0857017
H	-0.9181766	-0.1396977	3.0178403
H	-2.4208102	0.0088371	2.8659767
C	0.0983422	0.9567900	0.9757478
O	-0.7547616	1.8376006	0.7197399
O	0.5129242	0.5871264	2.1107359
H	0.3202168	-1.6645923	0.4158468
C	0.6914819	0.2572728	-0.2428093
N	1.1323166	-1.1281824	0.0672970
H	1.4914335	-1.5273926	-0.8100457
H	1.8727988	-1.1149341	0.7787947
H	1.5516798	0.8120659	-0.6111979
H	-0.0536525	0.1919756	-1.0231068
O	-3.2108877	-0.3131438	-0.5511631
H	-3.4164264	0.2641394	0.1993593
H	-2.6539981	-0.9988674	-0.1587550
O	-1.3497860	-2.0969132	0.9319246
H	-1.5414121	-1.6176872	1.7893046
H	-1.6544105	-2.9972774	1.0675905
O	2.0590080	-1.2052815	-2.5430015
H	1.4568274	-0.5391095	-2.9541828
H	2.2465632	-1.8361604	-3.2408712
O	3.8940283	0.6301318	-0.9269047
H	3.8368809	0.3211421	-0.0156173
H	3.5660589	-0.0948429	-1.4691507
O	-3.1618322	1.4013147	1.7865792
H	-2.2883496	1.7491848	1.4960400
H	-3.6712785	2.1645653	2.0654176
O	3.0472540	-0.2184264	1.8621784
H	3.5655149	-0.3843926	2.6517534
H	2.2072271	0.2009390	2.1630756
O	0.3383355	0.5970209	-3.5749766
H	0.6816726	1.3598845	-4.0436619
H	-0.4198938	0.9448164	-3.0490672

Table 64: Optimized Cartesian coordinates (in Angstrom) of the gw9-bb-1 structure, which corresponds to the Gly•$(H_2O)_9$ cluster after breaking the water bridge.

37
Energy=-971.0500178348

O	0.1599313	1.9370803	-2.9885888
H	-0.2023476	2.5690853	-3.6109217
H	-0.5063910	1.8481608	-2.2806221
O	-1.1517631	-1.3587033	3.1534000
H	-0.2543184	-1.0113083	2.9749118
H	-1.6421702	-0.5487217	3.3595510
C	0.9940469	0.7076928	1.4875647
O	0.1437074	1.6350097	1.5611018
O	1.1906034	-0.2424365	2.2781805
H	1.3710102	-1.1149919	-0.3987420
C	1.9207286	0.7265344	0.2625092
N	2.2515180	-0.6854921	-0.0413907
H	2.9955482	-0.7870433	-0.7530447
H	2.4641780	-1.1261949	0.8548961
H	2.8347325	1.2653618	0.4990523
H	1.4558501	1.1763070	-0.6084583
O	-3.4051823	0.3982207	0.5783783
H	-3.1679012	0.7547018	1.4496133
H	-3.1756157	-0.5410241	0.6444931
O	-2.1108321	-2.1869330	0.8470633
H	-1.7444449	-1.9485499	1.7432533
H	-2.5193583	-3.0483273	0.9528687
O	3.7166195	-0.6724899	-2.3344786
H	2.8756320	-0.6457334	-2.8476467
H	4.3335783	-1.1878084	-2.8554359
O	-1.2517876	1.3064144	-0.7679758
H	-2.1378871	1.0687003	-0.4076201
H	-0.7664556	1.6205056	0.0228970
O	-2.1125645	1.2903878	2.9637489
H	-1.2321177	1.4912712	2.5618809
H	-2.2883203	2.0044745	3.5791426
O	-0.2582602	-1.2553257	-0.9781719
H	-0.8749853	-1.7670186	-0.4189176
H	-0.6432417	-0.3512234	-0.9553909
O	1.2454201	-0.5753638	-3.3531448
H	0.6245972	-1.0695205	-2.8018083
H	0.8682435	0.3243016	-3.3721479

Table 65: Optimized Cartesian coordinates (in Angstrom) of the gw9-bb-20 structure, which corresponds to the Gly•$(H_2O)_9$ cluster after breaking the water bridge.

37
Energy=-971.0330622360

O	-0.7405822	1.6289681	-2.3218009
H	-1.2848686	2.1449272	-2.9198013
H	-1.2980339	1.5016789	-1.5120019
O	-2.2598642	-1.0935461	2.8509585
H	-1.2765823	-1.0357429	2.7861239
H	-2.5099073	-0.1631387	2.9551188
C	0.7763505	0.3022547	2.0547956
O	0.4239322	1.3489510	2.6362423
O	0.2978171	-0.8610137	2.1328757
H	1.2681779	-1.2959573	0.2321224
C	1.9478170	0.4618278	1.0827793
N	2.1818466	-0.8365718	0.3865749
H	2.6604577	-0.7207523	-0.5230755
H	2.7030774	-1.4704304	0.9829197
H	2.8509278	0.7548690	1.6096492
H	1.7313040	1.2137916	0.3282127
O	-2.2831219	1.1363968	-0.2343705
H	-2.2409128	1.4900123	0.6719465
H	-2.4448786	0.1881867	-0.1111940
O	-2.5021269	-1.6399444	0.3401958
H	-2.4801630	-1.4806717	1.3360621
H	-3.3033713	-2.1384582	0.1671696
O	2.9722995	-0.3996572	-2.2526349
H	2.0689824	-0.5656763	-2.6374856
H	3.6052191	-0.7351554	-2.8899142
O	1.9592646	2.3290379	-1.5843761
H	1.0478858	2.2264437	-1.8930835
H	2.4381258	1.6205768	-2.0264764
O	-2.1639202	1.7256558	2.5092905
H	-1.1862469	1.6318034	2.6679822
H	-2.4191745	2.5393126	2.9478982
O	-0.1064701	-2.3195020	-0.6959934
H	-0.9732576	-2.1133129	-0.2728556
H	-0.0553060	-3.2778321	-0.6844265
O	0.4807642	-0.7728970	-2.9751372
H	0.1371859	-1.3775915	-2.2982370
H	-0.0226474	0.0531575	-2.8460533

Table 66: Optimized Cartesian coordinates (in Angstrom) of the gw9-bb-21 structure, which corresponds to the Gly•$(H_2O)_9$ cluster after breaking the water bridge.

37
Energy=-971.0426976997

O	-0.8086392	1.8476340	-2.0627115
H	-1.0854336	2.6481797	-2.5112592
H	-1.5424946	1.6391740	-1.4373488
O	-1.9211127	-0.9407082	2.6755877
H	-0.9696353	-0.7211507	2.5548465
H	-2.3189361	-0.0650420	2.8018717
C	0.6701236	0.8454332	1.3540311
O	0.0883771	1.8968575	1.6754588
O	0.5707859	-0.3050513	1.8808589
H	1.3037055	-0.9870457	-0.4451394
C	1.6109644	0.9706077	0.1534731
N	2.1044247	-0.3576674	-0.2905369
H	2.6206783	-0.2752713	-1.1830100
H	2.6841961	-0.7854644	0.4429764
H	2.4637183	1.5908124	0.4149949
H	1.0718050	1.4354210	-0.6677095
O	-2.7968677	1.1491141	-0.3971024
H	-2.7662762	1.4990639	0.5088956
H	-2.7826344	0.1882719	-0.2737698
O	-2.4129782	-1.6302067	0.2248684
H	-2.2673661	-1.4224514	1.1983431
H	-3.1453863	-2.2492545	0.1935515
O	2.9319068	0.0622474	-2.8749499
H	2.0056443	-0.0577916	-3.1950595
H	3.5034889	-0.2626862	-3.5712617
O	3.0913304	-1.1965089	2.1676640
H	2.1476414	-0.9955348	2.3351139
H	3.3174657	-1.9341363	2.7354447
O	-2.4433202	1.8036412	2.3426717
H	-1.4627659	1.9025115	2.2223095
H	-2.7245190	2.5668542	2.8502111
O	-0.0946847	-2.0712114	-1.0878194
H	-0.9399638	-1.9526598	-0.5949321
H	0.0492015	-3.0199414	-1.1011021
O	0.3319045	-0.2969227	-3.3257750
H	0.0572953	-1.0069168	-2.7291977
H	-0.1416437	0.4877997	-2.9844879

Table 67: Optimized Cartesian coordinates (in Angstrom) of the gw9-bb-2 structure, which corresponds to the Gly•$(H_2O)_9$ cluster after breaking the water bridge.

37
Energy=-971.0336272737

O	-0.0444200	1.6021387	-3.3580246
H	-0.4197950	2.0769660	-4.1008457
H	-0.4855461	1.9726896	-2.5547405
O	-1.0939896	-1.5727273	2.1386845
H	-0.1866762	-1.3200287	2.3698859
H	-1.5662334	-0.7330658	2.3237736
C	1.0080171	0.7437286	1.1411156
O	0.3327291	1.7928392	1.2018207
O	1.2929175	-0.0576144	2.0772975
H	0.9158161	-1.5825053	-0.3407913
C	1.5704028	0.3684754	-0.2347824
N	1.8214356	-1.0939178	-0.2492988
H	2.4192898	-1.3876780	-1.0421612
H	2.2039848	-1.3234407	0.6704380
H	2.5112663	0.8866367	-0.4018255
H	0.8823179	0.6187471	-1.0328776
O	-2.9437230	0.4630591	-0.1050183
H	-2.9160448	0.6101598	0.8506461
H	-2.4891310	-0.3753407	-0.2350505
O	-0.8815832	-1.9911194	-0.4050291
H	-1.0301832	-1.8735266	0.5824113
H	-1.2124016	-2.8717962	-0.6027565
O	2.7712570	-1.6086137	-2.7203470
H	1.8488432	-1.4657067	-3.0291948
H	3.1709637	-2.2384593	-3.3209629
O	-1.1659175	2.3985351	-1.0899368
H	-1.8858629	1.8006872	-0.8207804
H	-0.5723810	2.3839789	-0.3193336
O	-1.9511409	1.0049034	2.5604763
H	-1.1933165	1.4331725	2.1142128
H	-1.6471472	1.0147980	3.4819154
O	0.0525937	0.7419176	4.5030919
H	0.6064984	0.5540086	3.7231897
H	0.5054222	1.4562692	4.9543827
O	0.1742970	-1.0574645	-3.0876923
H	-0.4283018	-1.2674720	-2.3667332
H	0.0257429	-0.1032337	-3.2751591

Table 68: Optimized Cartesian coordinates (in Angstrom) of the gw9-bb-3 structure, which corresponds to the Gly•$(H_2O)_9$ cluster after breaking the water bridge.

37
Energy=-971.0423072333

O	-0.2226838	1.6361681	-3.5273168
H	-0.5628285	2.1155822	-4.2845608
H	-0.7380172	1.9655684	-2.7571619
O	-1.0249687	-0.9365910	3.2988859
H	-0.2934907	-0.2949873	3.2365226
H	-1.7979745	-0.3975015	3.0712965
C	0.5552810	1.1126890	1.2217750
O	-0.3780025	1.9447315	1.1060449
O	1.0032613	0.6154885	2.2871033
H	1.2007367	-1.3096314	0.5394842
C	1.1954727	0.6468453	-0.0919879
N	1.8610306	-0.6681455	0.0711541
H	2.0729633	-1.0796127	-0.8569347
H	2.6991349	-0.5766470	0.6612612
H	1.9293486	1.3762169	-0.4274772
H	0.4357036	0.5483552	-0.8595226
O	-2.2463586	-0.6641573	-0.4388073
H	-2.6796013	-0.2065167	0.2987639
H	-1.6210514	-1.2553168	0.0127745
O	-0.3355170	-2.1421678	1.0679998
H	-0.6152430	-1.7908573	1.9598444
H	-0.4059660	-3.0981491	1.1230457
O	1.7756787	-1.8832289	-2.3652972
H	0.8595573	-1.6244284	-2.6248933
H	2.2773384	-1.8994078	-3.1816477
O	-1.6646283	2.0797550	-1.3114470
H	-1.9924954	1.1794534	-1.1780957
H	-1.1612301	2.2245262	-0.4858911
O	-2.7243128	0.8910477	1.9318480
H	-1.9214947	1.4264546	1.7463667
H	-3.4034910	1.5217681	2.1798849
O	3.5886273	-0.1339593	2.1673411
H	2.7254925	0.2302954	2.4526358
H	4.2509288	0.4989642	2.4487167
O	-0.6866087	-1.0065101	-2.9502159
H	-1.3750063	-0.9585081	-2.2749561
H	-0.5795849	-0.0875856	-3.2665361

Table 69: Optimized Cartesian coordinates (in Angstrom) of the gw9-bb-4 structure, which corresponds to the Gly•$(H_2O)_9$ cluster after breaking the water bridge.

37
Energy=-971.0400836926

O	-0.1148481	3.0422738	-3.4793613
H	-0.6718108	3.6349390	-3.9855524
H	-0.6797947	2.7144857	-2.7604770
O	-1.4372674	-1.2067188	3.0243336
H	-0.5899199	-0.7232058	3.0759926
H	-2.0800710	-0.4817899	2.9792405
C	0.6883275	0.6813034	1.3760835
O	-0.1954442	1.5442208	1.1500206
O	0.9024788	0.0790850	2.4618518
H	0.6729535	-1.5755657	0.1697516
C	1.5867613	0.2927780	0.1964650
N	1.6264464	-1.1904123	0.0648666
H	1.9925515	-1.4354010	-0.8763739
H	2.2166499	-1.5825670	0.8144278
H	2.6027162	0.6393009	0.3695998
H	1.2174997	0.7056009	-0.7345607
O	-3.1192092	-0.0827877	-0.2887479
H	-3.1900234	0.3797027	0.5602376
H	-2.5208880	-0.8177777	-0.0932801
O	-1.0641192	-2.0386785	0.5563241
H	-1.2432422	-1.8034011	1.5107402
H	-1.3415380	-2.9535858	0.4641511
O	2.3787453	-1.3376247	-2.5468613
H	1.7063545	-0.7300552	-2.9403965
H	2.4978403	-2.0420388	-3.1853558
O	-1.1811652	1.4724147	-1.4254298
H	-1.9914033	0.9790454	-1.1791647
H	-0.7781115	1.6475497	-0.5516073
O	-2.6316458	1.2164199	2.2326889
H	-1.7207892	1.4789661	1.9650235
H	-3.0052243	1.9783822	2.6792622
O	3.0848208	-1.4685382	2.3773662
H	3.2606086	-2.0561499	3.1136375
H	2.3456278	-0.8856551	2.6583952
O	0.4355217	0.2803705	-3.3465006
H	-0.1959636	0.5005556	-2.6368462
H	0.5365749	1.1445589	-3.7699445

Table 70: Optimized Cartesian coordinates (in Angstrom) of the gw9-bb-5 structure, which corresponds to the Gly•$(H_2O)_9$ cluster after breaking the water bridge.

37
Energy=-971.0400837079

O	0.2774592	3.0571926	-3.4572891
H	-0.2119811	3.6836141	-3.9918354
H	-0.3481859	2.7611971	-2.7758372
O	-1.6867788	-1.1292057	2.9237157
H	-0.8165748	-0.6979633	3.0296569
H	-2.2810260	-0.3666308	2.8456293
C	0.6439461	0.6329841	1.4200077
O	-0.1711866	1.5485645	1.1478406
O	0.7557418	0.0147597	2.5121149
H	0.5655319	-1.6141006	0.1979611
C	1.5868218	0.1954301	0.2934300
N	1.5450556	-1.2869300	0.1532837
H	1.9518250	-1.5499096	-0.7661387
H	2.0643880	-1.7170148	0.9338477
H	2.6095279	0.4791505	0.5296442
H	1.2998301	0.6334633	-0.6549113
O	-3.0954389	0.1070781	-0.4756036
H	-3.1892598	0.5698043	0.3710231
H	-2.5550359	-0.6633435	-0.2501282
O	-1.2163181	-1.9726384	0.4764125
H	-1.4381885	-1.7307170	1.4201477
H	-1.5423857	-2.8686338	0.3607210
O	2.4432350	-1.4689350	-2.4097782
H	1.8334966	-0.8203868	-2.8383983
H	2.5582162	-2.1767664	-3.0452400
O	-1.0024764	1.5465252	-1.4825234
H	-1.8543128	1.1021620	-1.2889199
H	-0.6429412	1.6935643	-0.5848658
O	-2.6834464	1.3647213	2.0802031
H	-1.7439703	1.5726795	1.8694901
H	-3.0366981	2.1462219	2.5092109
O	2.8421548	-1.6616560	2.5467649
H	2.1238299	-1.0361921	2.7874540
H	2.9381801	-2.2613007	3.2880336
O	0.6525213	0.2666382	-3.3123604
H	-0.0061732	0.5218437	-2.6401648
H	0.8306172	1.1247302	-3.7225983

Table 71: Optimized Cartesian coordinates (in Angstrom) of the gw9-bb-6 structure, which corresponds to the Gly•$(H_2O)_9$ cluster after breaking the water bridge.

37
Energy=-971.0500178215

O	0.1642032	1.9546451	-2.9771317
H	-0.1990102	2.5873445	-3.5982142
H	-0.5056184	1.8571032	-2.2736126
O	-1.1612000	-1.3839434	3.1389180
H	-0.2651355	-1.0293451	2.9678644
H	-1.6585080	-0.5785673	3.3465527
C	0.9801160	0.7064098	1.4974094
O	0.1228696	1.6273557	1.5708052
O	1.1785668	-0.2466216	2.2840473
H	1.3812548	-1.1033382	-0.3962950
C	1.9140125	0.7383938	0.2780983
N	2.2565721	-0.6696040	-0.0313777
H	3.0055379	-0.7620756	-0.7390727
H	2.4669720	-1.1136905	0.8637752
H	2.8227581	1.2823313	0.5230483
H	1.4512051	1.1895626	-0.5932514
O	-3.4111866	0.3713236	0.5597747
H	-3.1817248	0.7246950	1.4343573
H	-3.1755724	-0.5666779	0.6222382
O	-2.1006493	-2.2061074	0.8224186
H	-1.7412513	-1.9700758	1.7220638
H	-2.5037599	-3.0708917	0.9211125
O	3.7351329	-0.6337226	-2.3155706
H	2.8970771	-0.6099463	-2.8336453
H	4.3588970	-1.1416448	-2.8356794
O	-1.2561410	1.3016786	-0.7685029
H	-2.1427474	1.0559539	-0.4147932
H	-0.7777661	1.6148446	0.0269629
O	-2.1393326	1.2593940	2.9578006
H	-1.2579023	1.4685857	2.5623664
H	-2.3238104	1.9688390	3.5760003
O	-0.2434657	-1.2518631	-0.9863880
H	-0.8599672	-1.7708431	-0.4336409
H	-0.6348719	-0.3505849	-0.9610496
O	1.2694845	-0.5481665	-3.3486111
H	0.6488568	-1.0496682	-2.8037319
H	0.8861049	0.3489175	-3.3650458

Table 72: Optimized Cartesian coordinates (in Angstrom) of the gw9-bb-7 structure, which corresponds to the Gly•$(H_2O)_9$ cluster after breaking the water bridge.

37
Energy=-971.0329602368

O	0.0573168	2.7514823	-2.8621074
H	-0.3779436	3.4743241	-3.3173852
H	-0.6445055	2.2819752	-2.3761394
O	-1.2621690	-1.5656242	3.2920859
H	-0.4338526	-1.0474846	3.3234060
H	-1.9271138	-0.8646590	3.2076061
C	0.7412055	0.4022767	1.5204221
O	-0.1211419	1.3055959	1.2991940
O	0.9676705	-0.2080108	2.5842588
H	0.9185644	-1.9658331	0.5563362
C	1.5980987	-0.0241044	0.3277757
N	1.8334752	-1.4885290	0.4459943
H	2.2975881	-1.8289801	-0.4135673
H	2.3619267	-1.6691779	1.2950012
H	2.5514427	0.4957151	0.3327029
H	1.1132537	0.1606474	-0.6201377
O	-2.9758162	-0.6749683	-0.0117816
H	-3.0499237	-0.1702117	0.8134845
H	-2.3293983	-1.3620434	0.2021163
O	-0.7762167	-2.4818157	0.8857721
H	-0.9978440	-2.2121090	1.8250984
H	-1.0229275	-3.4079088	0.8208254
O	2.5431502	-1.7922380	-2.1549197
H	1.8909585	-1.1814932	-2.5675953
H	2.7384537	-2.4522178	-2.8212368
O	-1.1836676	0.9612242	-1.2338055
H	-1.9594161	0.4206668	-0.9725226
H	-0.7864892	1.1797048	-0.3643890
O	-2.5202814	0.7997683	2.3997407
H	-1.6299665	1.1234605	2.1250667
H	-2.9461741	1.5397915	2.8363808
O	1.6917249	2.9651404	-0.4142496
H	1.2256924	3.0469654	-1.2563192
H	0.9966566	2.7393590	0.2142860
O	0.6457491	-0.1075720	-3.0731520
H	-0.0799008	0.0796427	-2.4501233
H	0.8518209	0.7772406	-3.3981226

Table 73: Optimized Cartesian coordinates (in Angstrom) of the gw9-bb-8 structure, which corresponds to the Gly•$(H_2O)_9$ cluster after breaking the water bridge.

37
Energy=-971.0376895218

O	-0.3801147	1.6657616	-3.0675556
H	-0.3320932	2.4467008	-3.6203768
H	-0.8418116	1.9598139	-2.2410193
O	-1.1039812	-1.3348228	3.2763002
H	-0.2013696	-1.0209110	3.0815425
H	-1.5798062	-0.5044912	3.4397281
C	0.5451941	0.4698843	1.1540752
O	-0.0015285	1.5779727	1.3945456
O	1.0882600	-0.3213107	1.9627853
H	-0.0441896	-1.8867812	-0.0510999
C	0.5312508	0.0650931	-0.3195618
N	0.7426111	-1.3907374	-0.4967670
H	0.7742638	-1.5786049	-1.5001927
H	1.6495695	-1.6701094	-0.0598549
H	1.3208877	0.5941374	-0.8441561
H	-0.4222810	0.3217265	-0.7617570
O	-3.1706703	0.4585773	0.4701816
H	-3.0203996	0.7861427	1.3699964
H	-2.7791102	-0.4254130	0.4857337
O	-1.6502733	-2.0763893	0.8152649
H	-1.4888962	-1.8619105	1.7787018
H	-2.1561415	-2.8924149	0.8197930
O	3.5600348	-0.1283644	-1.7884333
H	2.8492313	-0.2255141	-2.4426015
H	4.1299128	0.5596075	-2.1360344
O	-1.5727758	2.3917921	-0.7931475
H	-2.2816103	1.7824819	-0.5156240
H	-0.9568670	2.3183118	-0.0389307
O	-2.0959086	1.2938974	3.0179956
H	-1.2548891	1.5332433	2.5634470
H	-2.2819719	2.0124001	3.6252641
O	3.2090104	-1.6495348	0.6382052
H	2.8207965	-1.0932153	1.3326178
H	3.6063478	-1.0389016	0.0015234
O	1.1487964	-0.5285605	-3.2248155
H	1.0490516	-0.8969112	-4.1052123
H	0.5914709	0.2873538	-3.2205612

Table 74: Optimized Cartesian coordinates (in Angstrom) of the gw9-bb-9 structure, which corresponds to the Gly•$(H_2O)_9$ cluster after breaking the water bridge.

37
Energy=-971.0382366908

O	-0.4287878	2.1438406	-3.6408051
H	-1.1134810	2.7829436	-3.8443634
H	-0.2860394	2.2179701	-2.6814055
O	-1.5315348	-1.2468502	3.1355285
H	-0.7374142	-0.7035103	3.3277108
H	-2.1645534	-0.5868125	2.8175614
C	0.8252528	1.0324768	2.2387464
O	-0.0953529	1.7153775	1.6835440
O	0.7319289	0.2585505	3.2030990
H	1.4475414	0.9319340	-0.3434441
C	2.2169576	1.1780794	1.5952671
N	2.1937563	0.5239222	0.2578386
H	3.0791033	0.6223497	-0.2291870
H	1.9891793	-0.5181187	0.3368917
H	2.9637128	0.6813558	2.2048625
H	2.4643199	2.2277950	1.4612416
O	-1.8230278	-0.4837119	-0.6626974
H	-2.3470609	-0.0023441	0.0002573
H	-1.5439699	-1.2887546	-0.1876683
O	-0.9238726	-2.5685983	0.9710790
H	-1.1514988	-2.1308024	1.8432048
H	-1.2884270	-3.4547232	1.0210946
O	1.6845685	-1.2978633	-2.3984633
H	0.8049638	-1.0517091	-2.7732283
H	2.1395858	-1.7348168	-3.1206161
O	-0.0470702	1.6118025	-0.9626152
H	-0.6287446	0.8218635	-0.9577117
H	-0.1508437	1.9324634	-0.0390047
O	-2.6260573	0.9184709	1.6460813
H	-1.7170257	1.2932228	1.7759367
H	-3.2355265	1.6211381	1.8798124
O	1.6941669	-2.0813500	0.2067615
H	0.8194705	-2.3573467	0.5384496
H	1.6151192	-2.0689799	-0.7657457
O	-0.7442811	-0.6174418	-3.3390938
H	-1.3607682	-0.6408915	-2.5945688
H	-0.7242890	0.3190690	-3.6043502

Table 75: Optimized Cartesian coordinates (in Angstrom) of the 2Za-1 zwitterionic structure, composed of the Gly•$(H_2O)_2$ cluster plus an extra water molecule bound to the NH_3^+ group.

19
Energy = -512.9769826594

C	-0.2277822	1.4498069	0.6961507
H	0.0753036	1.8939482	1.6413429
C	1.0118551	0.9844848	-0.0984756
N	-1.1242585	0.2926080	0.9785084
H	-0.7742083	2.1804146	0.1098688
O	1.3468491	-0.2367844	0.0809472
O	1.5219220	1.8214101	-0.8404782
H	-1.3303499	-0.1928953	0.0730992
H	-0.6421903	-0.3744586	1.6137046
H	-1.9965827	0.5914169	1.4021019
O	0.9599994	-0.8554632	-2.5069831
H	1.3426431	-0.7599844	-1.6075040
H	1.2760432	-0.0634233	-2.9511015
O	-1.5245437	-0.6534387	-1.5365334
H	-2.0025688	-1.4379025	-1.8116657
H	-0.6399214	-0.7262136	-1.9784518
O	0.5414519	-1.4348290	2.2541539
H	1.0526175	-1.0933524	1.4752011
H	1.1337208	-1.3853442	3.0061146

Table 76: Optimized Cartesian coordinates (in Angstrom) of the 2Za-2 zwitterionic structure, composed of the Gly•$(H_2O)_2$ cluster plus an extra water molecule bound to the NH_3^+ group.

19
Energy = -512.9686154015

C	0.1597248	1.1736288	0.2866663
H	0.1556174	1.8283367	1.1530221
C	1.6077067	0.7070296	-0.0256315
N	-0.5959473	-0.0661079	0.5974299
H	-0.2693327	1.6826877	-0.5683045
O	1.8126621	-0.5098695	0.3227035
O	2.3565982	1.5080959	-0.5764715
H	-1.0221813	-0.4355598	-0.2646530
H	0.2342639	-0.6979074	0.7942544
H	-1.2537057	0.0213482	1.3704783
O	1.7777359	-1.3718417	-2.2503883
H	1.9887199	-1.2079871	-1.3060375
H	2.2912970	-0.6970384	-2.7024582
O	-0.8754553	-0.8832144	-2.0098660
H	-1.3687268	-1.4892641	-2.5642617
H	0.0736838	-1.0748069	-2.1976586
O	-2.2527081	0.3517786	2.9695419
H	-1.9362003	0.1040933	3.8412431
H	-2.8837523	1.0565983	3.1303912

Table 77: Optimized Cartesian coordinates (in Angstrom) of the 3Za-1 zwitterionic structure, composed of the Gly•$(H_2O)_3$ cluster plus an extra water molecule bound to the NH_3^+ group.

22
Energy = -589.3170254788

C	-0.5864421	-0.2803719	1.0940094
H	-0.7375356	-0.5833052	2.1268523
C	-0.4058833	1.2537907	1.0156751
N	0.6899404	-0.8516464	0.5967885
H	-1.4073088	-0.6262472	0.4761421
O	0.7859706	1.6244326	1.2084914
O	-1.4135848	1.9360936	0.7550345
H	0.8488610	-1.8265132	0.8541330
H	0.6876259	-0.6940690	-0.4453298
H	1.3960326	-0.2074660	0.9803177
O	-2.3156950	0.6715220	-1.4368955
H	-2.1512315	1.2176697	-0.6334288
H	-2.9302142	1.1782779	-1.9697998
O	0.3558892	0.0237654	-1.9146906
H	-0.5964356	0.2367053	-1.9357587
H	0.7860629	0.9012544	-1.8523428
O	1.5054993	2.4616787	-1.2644162
H	1.2926461	2.3683681	-0.3119232
H	1.0815463	3.2825100	-1.5219391
O	0.9436667	-3.6510149	1.3666063
H	1.5349603	-4.0636416	1.9997833
H	0.6356295	-4.3717929	0.8126907

Table 78: Optimized Cartesian coordinates (in Angstrom) of the 3Za-2 zwitterionic structure, composed of the Gly•$(H_2O)_3$ cluster plus an extra water molecule bound to the NH_3^+ group.

22
Energy = -589.3262805905

C	-0.7313119	-0.7592782	1.1679272
H	-0.6772089	-0.9475555	2.2376584
C	-0.5355307	0.7443896	0.8869271
N	0.3598348	-1.5203457	0.4940013
H	-1.6819880	-1.1002410	0.7728182
O	0.6420768	1.1784567	1.0633718
O	-1.5269276	1.3827486	0.4935920
H	0.1987009	-2.5207143	0.5450288
H	0.3789702	-1.2105647	-0.5256458
H	1.2675806	-1.3022061	0.9487782
O	-2.5238389	-0.1404735	-1.4650007
H	-2.3462042	0.5053021	-0.7438444
H	-3.2523908	0.2241437	-1.9698110
O	0.1668704	-0.5330487	-1.9606925
H	-0.7951213	-0.3790857	-2.0187647
H	0.5573247	0.3665227	-1.9347603
O	1.2093823	1.9707586	-1.4735360
H	1.0398901	1.9052348	-0.5111115
H	0.6991443	2.7347219	-1.7500629
O	2.3810064	-0.5417683	2.0454582
H	3.3027073	-0.3230100	1.8970304
H	1.8670333	0.2660130	1.8006381

Table 79: Optimized Cartesian coordinates (in Angstrom) of the 4Za-1 zwitterionic structure, composed of the Gly•$(H_2O)_4$ cluster plus an extra water molecule bound to the NH_3^+ group.

25
Energy = -665.6696565394

C	-0.1110429	0.0582987	1.4653954
H	0.3078303	0.3180593	2.4337728
C	-0.3085258	1.3169219	0.6065566
N	0.8551758	-0.8409707	0.7669300
H	-1.0409921	-0.4804504	1.5962712
O	0.7326427	2.0048787	0.4041256
O	-1.4500412	1.5237283	0.1413129
H	0.6853259	-1.8068158	1.0429401
H	0.6819933	-0.7899651	-0.2721284
H	1.8154740	-0.5201412	0.9644347
O	-2.4136639	-0.7668895	-0.6905399
H	-3.3372245	-0.7160130	-0.9447786
H	-2.1855924	0.1321057	-0.3233838
O	0.2056013	-0.6027055	-1.8516468
H	0.3570252	0.3242168	-2.1401795
H	-0.7570081	-0.6884622	-1.7987630
O	0.6481079	2.0680208	-2.3121246
H	-0.1194589	2.5567157	-2.6170006
H	0.6804265	2.2639530	-1.3522438
O	2.8899312	0.8389088	1.4526475
H	2.2134551	1.4546637	1.0813974
H	3.7343956	1.1383180	1.1123702
O	-1.1076310	-2.8357310	0.6949797
H	-1.2869639	-3.7112869	0.3491326
H	-1.6892402	-2.2393582	0.1905222

Table 80: Optimized Cartesian coordinates (in Angstrom) of the 5Za-1 zwitterionic structure, composed of the Gly•$(H_2O)_5$ cluster plus an extra water molecule bound to the NH_3^+ group.

28
Energy = -742.0093304275

C	-0.8648523	1.6895475	-0.7332046
H	-0.2735670	2.5917647	-0.8432095
C	-0.3458221	0.5880155	-1.6740513
N	-0.7278635	1.1966266	0.6651265
H	-1.9151390	1.8985918	-0.9191075
O	-0.9801125	-0.5027357	-1.6289965
O	0.6720003	0.8649769	-2.3433150
H	-1.3599445	0.3752971	0.8163796
H	0.2409204	0.8323190	0.8159392
H	-0.9425314	1.9292029	1.3451616
O	-2.2052097	-1.1059156	0.7310829
H	-2.0094556	-1.0476675	-0.2255708
H	-1.5402261	-1.7456280	1.0328073
O	2.6752949	-0.6791918	-1.6197461
H	3.4993434	-0.4831312	-2.0691298
H	1.9911237	-0.1102495	-2.0530618
O	1.6659487	-0.1078315	0.9672542
H	1.3169024	-0.9964345	1.1560847
H	2.1709413	-0.2292905	0.1439659
O	0.2485197	-2.5428047	1.1063591
H	0.4081837	-2.7033838	0.1351428
H	0.4522069	-3.3725114	1.5425200
O	0.6441439	-2.6834511	-1.4948564
H	1.5048349	-2.2742576	-1.6645594
H	0.0207281	-1.9721769	-1.7559105
O	-1.3917646	3.3647539	2.5063533
H	-2.2037750	3.3890151	3.0176420
H	-0.7508290	3.8365501	3.0429000

Table 81: Optimized Cartesian coordinates (in Angstrom) of the 6Za-1 zwitterionic structure, composed of the Gly•$(H_2O)_6$ cluster plus an extra water molecule bound to the NH_3^+ group.

31
Energy = -818.3535638147

C	1.4362159	-0.1038453	1.3691082
H	1.6350519	0.8963652	1.7398232
C	-0.0497368	-0.4605896	1.5361643
N	1.8054817	-0.1572626	-0.0672334
H	2.0437808	-0.8239530	1.9119555
O	-0.7586032	0.3772796	2.1490398
O	-0.4086833	-1.5566589	1.0390968
H	2.8019230	0.0298336	-0.2033020
H	1.5620457	-1.0779158	-0.4916362
H	1.2349944	0.5556445	-0.5977603
O	-1.1967877	-0.7153031	-2.3993426
H	-1.8692328	-0.9017778	-1.6889974
H	-1.6717300	-0.7922537	-3.2292971
O	0.8179745	-2.4563056	-1.2681227
H	0.3154849	-2.5052980	-0.4370071
H	0.1831694	-2.0244692	-1.8625470
O	-2.7490481	-1.2910558	-0.3533273
H	-2.0240907	-1.5209780	0.2620557
H	-3.1992970	-0.5761214	0.1237192
O	0.1749232	1.5164949	-1.3927209
H	-0.4038342	0.8756802	-1.8421759
H	-0.4021031	2.0045938	-0.7680812
O	-3.3437060	0.7693624	1.4811143
H	-3.9851352	0.6861713	2.1890730
H	-2.4815216	0.5086636	1.8766700
O	-1.2373932	2.6762215	0.6513751
H	-0.9264579	2.0395792	1.3182821
H	-2.1870792	2.5094601	0.6655142
O	4.6482093	0.4344152	-0.3474518
H	4.9416027	1.2814397	-0.6912771
H	5.2935827	-0.1974172	-0.6727112

Table 82: Optimized Cartesian coordinates (in Angstrom) of the 7Zb-1 zwitterionic structure, composed of the Gly•$(H_2O)_7$ cluster plus an extra water molecule bound to the NH_3^+ group.

34
Energy = -894.6981218630

C	0.4648697	-0.6975648	2.2546282
H	0.7078565	-1.7501267	2.3528786
C	1.4418566	-0.0361399	1.2718961
N	-0.9361330	-0.5675723	1.7905151
H	0.5570617	-0.2194139	3.2275827
O	2.5500486	-0.5830864	1.1560431
O	1.0133099	1.0095939	0.6915086
H	-1.2055740	0.4314688	1.6640086
H	-1.0405031	-1.0007234	0.8408550
H	-1.5852408	-1.0158935	2.4411779
O	-1.2929769	-1.4835713	-0.7438826
H	-0.4930570	-1.5710816	-1.2959008
H	-1.7369436	-0.6967686	-1.1041301
O	0.9258201	-1.4169225	-2.4363698
H	1.1138984	-2.1152956	-3.0665510
H	1.8148437	-1.1500554	-2.0640079
O	3.2053734	-0.5452467	-1.4777726
H	3.1229712	-0.5828036	-0.5002485
H	3.1515379	0.4061190	-1.6493666
O	2.1902844	2.1079948	-1.3907654
H	1.8312402	1.7481091	-0.5360179
H	2.5749234	2.9603126	-1.1792236
O	-2.1906468	1.0883403	-1.5082197
H	-1.3724448	1.2276967	-2.0577452
H	-2.9210093	1.3414822	-2.0764336
O	-1.4867325	2.0551816	1.0919269
H	-1.8707878	1.8993911	0.2136359
H	-0.5303344	1.9763637	0.9181306
O	0.0273581	1.2323348	-2.9238499
H	0.3361892	0.3114773	-2.9425597
H	0.7567900	1.7046509	-2.4852257
O	-2.6948878	-1.8952694	3.7130295
H	-3.1140805	-2.7387356	3.5278837
H	-3.3148808	-1.4342457	4.2825703

Table 83: Optimized Cartesian coordinates (in Angstrom) of the 8Za-1 zwitterionic structure, composed of the Gly•$(H_2O)_8$ cluster plus an extra water molecule bound to the NH_3^+ group.

37
Energy = -971.0432343223

C	2.2570808	0.1034827	0.8108190
H	2.4377846	1.1250809	1.1290443
C	0.9080454	-0.3889776	1.3536650
N	2.2921939	0.0572980	-0.6693052
H	3.0425182	-0.5394502	1.2023052
O	0.3865604	0.3050910	2.2536126
O	0.4766960	-1.4655802	0.8538363
H	3.2311051	0.2558664	-1.0230643
H	1.9636601	-0.8542593	-1.0448204
H	1.6148340	0.7796971	-1.0497989
O	-1.9852645	-2.3762767	1.2392503
H	-1.9627845	-3.3322826	1.3098734
H	-1.0401734	-2.0862496	1.1648100
O	0.9935556	-2.1583092	-1.7723905
H	0.6896251	-2.2208184	-0.8519140
H	0.2749328	-1.6609995	-2.1977086
O	-2.2344979	-0.1516413	2.9693914
H	-2.3664507	-1.0433717	2.6164788
H	-1.2706464	-0.0228000	2.8493066
O	-0.6093925	2.5636894	0.8273736
H	-0.2122623	1.9412922	1.4576535
H	-1.5568552	2.3582168	0.8859144
O	-2.9649221	-0.6630297	-0.7623706
H	-2.7278064	-1.3600509	-0.1274870
H	-3.1471957	0.1122573	-0.2047379
O	-3.2013280	1.4455248	1.1072121
H	-2.9180133	0.8790430	1.8750598
H	-4.0062648	1.8848556	1.3883394
O	0.4627421	1.7907022	-1.5352696
H	-0.1773739	1.1928494	-1.9591401
H	0.0079503	2.1430583	-0.7359361
O	-1.0725644	-0.3302543	-2.5642101
H	-1.8005784	-0.4566340	-1.8972860
H	-1.5164352	-0.3174667	-3.4148224
O	4.9919267	0.7295625	-1.5464352
H	5.1707601	1.6094604	-1.8864993
H	5.5688381	0.1514238	-2.0507493

Table 84: Cartesian coordinates (in Angstrom) of the optimized gw10-rb-10 structure, which corresponds to the Gly•$(H_2O)_{10}$ cluster after removing the exo bond.

40
Energy=-1047.3893059901

O	3.1921721	0.4001589	-2.4284188
H	4.0752631	0.1468002	-2.7025408
H	2.8834369	-0.3095659	-1.8140868
O	-0.9167573	-1.1384240	3.6071850
H	-1.5983942	-1.6126799	3.1040473
H	-1.1756054	-0.2025265	3.5080325
C	0.9245628	-1.4766891	-0.5969646
O	2.1522411	-1.2485245	-0.6162722
O	0.1226363	-1.5496055	-1.5719931
H	1.2682137	-0.1319135	1.6443029
C	0.2987123	-1.7070462	0.7742803
N	1.1564412	-1.1603334	1.8453531
H	0.6306713	-1.2574586	2.7366786
H	2.0686828	-1.6031210	1.8405028
H	0.1272625	-2.7672551	0.9441254
H	-0.6515129	-1.1946438	0.8502689
O	-1.4357767	1.5425659	2.9329707
H	-1.8015434	1.5721768	2.0378534
H	-0.5528927	1.9061789	2.7989653
O	-1.5998790	1.2885281	0.0112887
H	-1.9892233	0.4662321	-0.3303349
H	-1.3334306	1.7846733	-0.7859941
O	-0.3802722	2.4621292	-2.1914505
H	-0.0666605	1.6905189	-2.7371922
H	-0.7636129	3.0826257	-2.8147069
O	2.2032083	2.5648776	-0.8742401
H	2.6838659	1.9126345	-1.4093556
H	1.4035383	2.7463021	-1.3897989
O	0.9242255	1.4235797	1.2063056
H	0.0648426	1.3469356	0.7493566
H	1.5029927	1.8490078	0.5296389
O	-2.7368316	-2.3767427	1.7653769
H	-2.7422581	-2.0679709	0.8431097
H	-3.6574164	-2.5325541	1.9833878
O	-2.3805819	-1.3059500	-0.8427009
H	-1.4593012	-1.4858164	-1.1884204
H	-2.9702708	-1.4691280	-1.5824540
H	1.5448463	0.4447589	-3.4356259
O	0.5794982	0.3716775	-3.4849924
H	0.4049069	-0.4044124	-2.9154876

Table 85: Cartesian coordinates (in Angstrom) of the optimized gw10-rb-11 structure, which corresponds to the Gly•$(H_2O)_{10}$ cluster after removing the exo bond.

40
Energy=-1047.3817211832

O	3.2067082	0.5057789	-1.9943542
H	4.1650461	0.5060455	-1.9657975
H	2.9171107	-0.2351850	-1.4037247
O	-1.2395356	-0.6027017	3.6359197
H	-1.7993187	-0.2868147	2.9120018
H	-0.8122291	0.2046554	3.9684630
C	0.9871564	-1.6193657	-0.5004588
O	2.1809447	-1.2773684	-0.3240098
O	0.3533206	-1.7402927	-1.5801722
H	0.7991217	-0.1441805	1.6158876
C	0.2045291	-1.9336060	0.7763815
N	0.7865034	-1.1519593	1.8921992
H	0.1830963	-1.1966200	2.7349738
H	1.7465368	-1.4376541	2.0548512
H	0.2827841	-2.9940754	1.0041881
H	-0.8478959	-1.6836295	0.6880308
O	0.5331045	1.5245472	4.0034677
H	0.6399171	2.3250248	4.5191588
H	0.6106168	1.7949728	3.0711147
O	-2.2206898	0.7230326	1.1487023
H	-2.1574816	0.3477713	0.2385466
H	-3.1117431	1.0748226	1.2083712
O	-0.6065450	1.5953274	-3.0259042
H	0.0300086	0.9276536	-3.4041306
H	-0.9231176	2.1063779	-3.7734732
O	1.3167669	2.3774021	-1.0528606
H	2.0650241	1.8424660	-1.3686127
H	0.6386196	2.2626178	-1.7379031
O	0.4127878	1.5015773	1.2826793
H	-0.5547108	1.4810335	1.1778876
H	0.7721866	1.8629919	0.4302298
O	-3.3124045	-2.2283008	0.0011400
H	-3.0707787	-1.6098915	-0.7011521
H	-3.5398218	-3.0359214	-0.4624331
O	-1.8798609	-0.2462448	-1.3525397
H	-1.1261962	-0.8722891	-1.4545947
H	-1.6580806	0.4646217	-1.9802124
H	1.9952220	0.0516958	-3.4510136
O	1.1249204	-0.2511211	-3.7497699
H	0.9083771	-0.9331945	-3.0810774

Table 86: Cartesian coordinates (in Angstrom) of the optimized gw10-rb-12 structure, which corresponds to the Gly•$(H_2O)_{10}$ cluster after removing the exo bond.

40
Energy=-1047.3919917230

O	2.6069156	0.8435544	-2.2070701
H	3.5592930	0.9515804	-2.2293674
H	2.4331337	0.0716869	-1.6150859
O	-1.7263607	-0.7810615	3.4224600
H	-2.2806437	-0.5050934	2.6766194
H	-1.4005060	0.0596291	3.7860214
C	0.7148384	-1.5561840	-0.6271422
O	1.8861486	-1.0915581	-0.5155060
O	0.0595136	-1.7336709	-1.6761469
H	0.4430225	-0.1438600	1.5310007
C	0.0172712	-1.9640969	0.6736669
N	0.4766792	-1.1408529	1.8158658
H	-0.2020241	-1.2154680	2.5968870
H	1.4343934	-1.3980425	2.0858621
H	0.2326715	-3.0092235	0.8847037
H	-1.0563773	-1.8418185	0.5756878
O	-0.2677196	1.5647809	3.8398442
H	-0.3095033	2.3944541	4.3171855
H	-0.1913824	1.8021598	2.8979085
O	-2.8151246	0.3236735	0.9664096
H	-2.7302554	-0.0262510	0.0375112
H	-3.6839588	0.7297699	1.0022861
O	-1.3010566	1.4811524	-3.1307858
H	-0.6155006	0.8781222	-3.5272905
H	-1.7154943	1.9276887	-3.8717811
O	0.5286318	2.4921561	-1.1991058
H	1.3301068	2.0556896	-1.5311303
H	-0.1383879	2.3022247	-1.8788785
O	-0.2658807	1.4385185	1.1180130
H	-1.2105675	1.2424072	0.9862041
H	0.0429189	1.8665618	0.2795518
O	3.0637320	-2.1111029	1.6974389
H	2.9037902	-1.7530381	0.8010767
H	3.9661548	-1.8823094	1.9243563
O	-2.4217752	-0.5241111	-1.4921803
H	-1.6461025	-1.1093600	-1.5828047
H	-2.1998462	0.2182540	-2.0803837
H	1.4226323	0.2176729	-3.6236389
O	0.5893780	-0.1895847	-3.9022422
H	0.4672419	-0.8850498	-3.2260204

Table 87: Cartesian coordinates (in Angstrom) of the optimized gw10-rb-13 structure, which corresponds to the Gly•$(H_2O)_{10}$ cluster after removing the exo bond.

40
Energy=-1047.3882103974

O	2.7453081	0.8302923	-1.9621087
H	3.6974094	0.9125120	-1.8835276
H	2.4854956	0.0736734	-1.3776948
O	-2.0026451	-0.6376227	3.3994585
H	-2.4750556	-0.2857372	2.6294442
H	-1.4375419	0.0869827	3.6963085
C	0.7746073	-1.6789303	-0.6189697
O	1.8010399	-1.0154801	-0.3061040
O	0.3223132	-1.9257859	-1.7598013
H	-0.0505252	-0.3626202	1.3724094
C	-0.0310300	-2.2496573	0.5542735
N	0.0810331	-1.3364459	1.7088567
H	-0.6422454	-1.4725674	2.4283508
H	1.0272389	-1.3515084	2.1274880
H	0.3587517	-3.2276319	0.8263585
H	-1.0771786	-2.3493635	0.2845691
O	0.5105906	1.1755497	3.4791649
H	0.6529724	1.9530733	4.0231023
H	0.1921959	1.5080331	2.6154365
O	-2.9702988	0.2529614	0.7948191
H	-2.7194744	-0.1439082	-0.0791007
H	-3.8888542	0.5121286	0.6948384
O	-1.0749622	1.3228638	-3.2390204
H	-0.3344954	0.7447300	-3.5743769
H	-1.4663771	1.7251527	-4.0169204
O	0.5479626	2.4195436	-1.2004839
H	1.3957387	2.0149570	-1.4505213
H	-0.0419510	2.2066652	-1.9426044
O	-0.4378796	1.3317468	0.9920798
H	-1.3975919	1.2745664	0.8590721
H	-0.0607451	1.7487876	0.1706976
O	2.6590849	-0.7019411	2.4522858
H	2.2885506	0.1186715	2.8031879
H	2.6767664	-0.5880895	1.4898173
O	-2.1810477	-0.6564649	-1.5776224
H	-1.4248570	-1.2595335	-1.6938614
H	-1.9597862	0.0796774	-2.1750585
H	1.7255486	0.1812278	-3.4941235
O	0.9364764	-0.2544084	-3.8484817
H	0.7954578	-0.9761001	-3.2016371

Table 88: Cartesian coordinates (in Angstrom) of the optimized gw10-rb-14 structure, which corresponds to the Gly•$(H_2O)_{10}$ cluster after removing the exo bond.

40
Energy=-1047.3919916445

O	2.6078348	0.8312262	-2.2107911
H	3.5621276	0.9194179	-2.2381698
H	2.4219703	0.0517932	-1.6325236
O	-1.7171085	-0.8107609	3.4202547
H	-2.2710528	-0.5087261	2.6843395
H	-1.3706951	0.0156303	3.7972936
C	0.6767524	-1.5584543	-0.6628399
O	1.8583865	-1.1206801	-0.5513252
O	0.0101308	-1.7017246	-1.7099341
H	0.4509508	-0.1831267	1.5242884
C	-0.0196294	-1.9769414	0.6352703
N	0.4655144	-1.1859784	1.7895288
H	-0.2087935	-1.2614171	2.5742706
H	1.4195141	-1.4685165	2.0470759
H	0.1751321	-3.0302841	0.8243118
H	-1.0911352	-1.8302138	0.5479671
O	-0.2055585	1.4950706	3.8712967
H	-0.2256545	2.3159519	4.3649470
H	-0.1311094	1.7490230	2.9335352
O	-2.8004393	0.3641996	0.9944818
H	-2.7299454	0.0307919	0.0583231
H	-3.6600313	0.7880244	1.0449605
O	-1.2923157	1.5691416	-3.0909897
H	-0.6226505	0.9596547	-3.5045128
H	-1.7026873	2.0388083	-3.8198393
O	0.5727840	2.5033605	-1.1544732
H	1.3623148	2.0566222	-1.5011341
H	-0.1031497	2.3408644	-1.8325337
O	-0.2268875	1.4217585	1.1477282
H	-1.1764705	1.2482836	1.0194976
H	0.0848436	1.8592996	0.3152345
O	3.0302520	-2.2081963	1.6320943
H	2.8715256	-1.8292030	0.7441785
H	3.9392044	-2.0039052	1.8562868
O	-2.4433107	-0.4436136	-1.4830173
H	-1.6810297	-1.0433433	-1.5910547
H	-2.2098754	0.3052317	-2.0584169
H	1.3999437	0.2582400	-3.6296380
O	0.5561182	-0.1256299	-3.9096337
H	0.4242298	-0.8316788	-3.2463378

Table 89: Cartesian coordinates (in Angstrom) of the optimized gw10-rb-1 structure, which corresponds to the Gly•$(H_2O)_{10}$ cluster after removing the exo bond.

40
Energy=-1047.3920866702

O	2.6735912	0.7830946	-2.1536640
H	3.6295063	0.8557620	-2.1327166
H	2.4487695	0.0019656	-1.5940211
O	-1.7750114	-0.7983576	3.3867736
H	-2.3102143	-0.4641250	2.6508980
H	-1.4128491	0.0099131	3.7880650
C	0.6132914	-1.5667068	-0.6789934
O	1.8121348	-1.1829842	-0.5582947
O	-0.0499904	-1.6804551	-1.7318695
H	0.4604766	-0.2149793	1.5383842
C	-0.1150263	-1.9551655	0.6110925
N	0.4155087	-1.2223949	1.7825143
H	-0.2681989	-1.2742261	2.5617075
H	1.3496499	-1.5670687	2.0368172
H	-0.0008762	-3.0236149	0.7808691
H	-1.1730951	-1.7323895	0.5213343
O	-0.2157223	1.4499414	3.9003289
H	-0.1666467	2.2566217	4.4146738
H	-0.0999708	1.7165694	2.9706582
O	-2.7878282	0.4620163	0.9726418
H	-2.7265198	0.1475666	0.0295527
H	-3.6261152	0.9260596	1.0278560
O	-1.1871087	1.6664702	-3.0823033
H	-0.5330860	1.0378666	-3.4913825
H	-1.5648740	2.1611744	-3.8122281
O	0.6814050	2.5081524	-1.1033927
H	1.4592905	2.0384698	-1.4464768
H	0.0094557	2.3796002	-1.7923468
O	-0.1717496	1.4139427	1.1739204
H	-1.1255151	1.2776607	1.0334832
H	0.1621118	1.8568791	0.3530632
O	3.0575950	-2.0803243	1.6613374
H	2.8230835	-1.8225137	0.7463622
H	3.5288768	-2.9119368	1.5915990
O	-2.4483391	-0.3131231	-1.5191505
H	-1.7137639	-0.9459955	-1.6280752
H	-2.1734976	0.4324271	-2.0805583
H	1.4669458	0.2595499	-3.5964696
O	0.6124115	-0.0877215	-3.8910494
H	0.4418947	-0.7976213	-3.2409402

Table 90: Cartesian coordinates (in Angstrom) of the optimized gw10-rb-21 structure, which corresponds to the Gly•$(H_2O)_{10}$ cluster after removing the exo bond.

40
Energy = -1043.669720205

O	1.7220961	1.9376313	-2.1345956
H	2.5650177	2.3622770	-2.3062462
H	1.9243593	0.9851874	-1.9702512
O	-2.2309740	0.3960272	2.1929628
H	-2.5128349	0.6247660	1.2938421
H	-1.6931086	1.1557739	2.4734477
C	0.6556765	-1.0650260	-1.4629079
O	1.8468842	-0.6179247	-1.3938749
O	-0.0120097	-1.2851096	-2.4864264
H	0.4863389	0.4158148	0.7744570
C	-0.0280176	-1.3633068	-0.1260382
N	0.6103141	-0.5908990	0.9711377
H	0.1943085	-0.8340283	1.8802457
H	1.6122938	-0.8038594	1.0013018
H	0.0563355	-2.4214284	0.1106689
H	-1.0765196	-1.0862779	-0.1683938
O	-0.3051191	2.3520491	2.7435858
H	-0.3527194	3.2088445	3.1706918
H	-0.0502250	2.5275563	1.8212398
O	-2.5523799	1.4434116	-0.4548708
H	-2.5330578	0.9450190	-1.3253048
H	-3.2826726	2.0612007	-0.5367264
O	3.1202349	-1.8410905	0.6284222
H	2.8868540	-1.4913254	-0.2595888
H	4.0768279	-1.8135194	0.6867826
O	1.0527260	-3.7195391	1.7969242
H	0.5657479	-3.1893134	2.4353154
H	1.8596815	-3.2277478	1.6077884
O	0.0671566	2.0324934	0.0740077
H	-0.8538554	1.9721727	-0.2498356
H	0.6377944	2.1835506	-0.7038923
O	-0.7629925	-1.6210742	3.2136703
H	-0.7078669	-1.4929857	4.1630429
H	-1.4846447	-1.0253300	2.9192709
O	-2.3532752	0.1594185	-2.7073933
H	-1.7746232	-0.6099905	-2.5645359
H	-1.7940983	0.6762126	-3.3179297
H	0.4564219	1.5555690	-3.6907563
O	-0.1515718	0.9967403	-4.1912584
H	0.1154964	0.1080602	-3.9079792

Table 91: Cartesian coordinates (in Angstrom) of the optimized gw10-rb-2 structure, which corresponds to the Gly•$(H_2O)_{10}$ cluster after removing the exo bond.

40
Energy=-1047.3919917298

O	2.7755274	0.4649552	-2.1115896
H	3.7292091	0.3670831	-2.1218198
H	2.4274191	-0.3032278	-1.5966688
O	-1.9292878	-0.7070543	3.3288877
H	-2.3948990	-0.2499297	2.6120154
H	-1.4392123	0.0061413	3.7719327
C	0.3789452	-1.6080910	-0.7722999
O	1.6197821	-1.4189271	-0.6146490
O	-0.2756534	-1.5417077	-1.8345852
H	0.3677696	-0.3780467	1.5108945
C	-0.4185607	-1.9758749	0.4822237
N	0.1808744	-1.3810444	1.6988781
H	-0.5152764	-1.3803788	2.4680170
H	1.0550797	-1.8623701	1.9445635
H	-0.4366433	-3.0578897	0.5924060
H	-1.4386890	-1.6167932	0.3946152
O	-0.0119675	1.2205340	3.9717561
H	0.1141889	1.9915223	4.5263891
H	0.1343691	1.5227219	3.0570498
O	-2.7014066	0.8302923	0.9882567
H	-2.6727365	0.5585474	0.0302177
H	-3.4637685	1.4086708	1.0614597
O	-0.8838087	2.0119229	-2.9764910
H	-0.3345549	1.3151730	-3.4278440
H	-1.1764637	2.6043241	-3.6719325
O	1.0763878	2.4207642	-0.9536571
H	1.7730538	1.8549634	-1.3246488
H	0.3994900	2.4430876	-1.6496353
O	0.0233778	1.3512869	1.2503741
H	-0.9382155	1.3762608	1.0987791
H	0.4352399	1.7791589	0.4573426
O	2.5022047	-2.8699669	1.4922733
H	2.4426446	-2.4038226	0.6341278
H	3.4274045	-2.8630230	1.7415957
O	-2.4439920	0.1509102	-1.5396488
H	-1.8097410	-0.5764796	-1.6846663
H	-2.0552524	0.8796877	-2.0535606
H	1.5165885	0.2435466	-3.5836729
O	0.6218835	0.0529749	-3.9014418
H	0.3386894	-0.6599021	-3.2952446

Table 92: Cartesian coordinates (in Angstrom) of the optimized gw10-rb-3 structure, which corresponds to the Gly•$(H_2O)_{10}$ cluster after removing the exo bond.

40
Energy=-1047.3833997484

O	2.5360842	0.4635793	-1.9056035
H	3.4029398	0.0814871	-2.0880255
H	2.1324055	-0.2297295	-1.3443955
O	-1.6233275	-0.6128238	3.7652236
H	-2.1876530	-0.2091721	3.0893835
H	-1.1200900	0.1381429	4.1232419
C	0.2092493	-1.7585739	-0.5110554
O	1.4543333	-1.5738465	-0.4189748
O	-0.5005306	-1.8205303	-1.5379956
H	0.3349136	-0.2380784	1.6390736
C	-0.5111822	-1.9349442	0.8275415
N	0.2590833	-1.2507727	1.8898274
H	-0.2623164	-1.2692745	2.7852728
H	1.1973873	-1.6358936	1.9390424
H	-0.5891824	-2.9930827	1.0659175
H	-1.5066629	-1.5064055	0.8034695
O	0.3001855	1.3643164	4.1031358
H	0.5325435	2.1304409	4.6296033
H	0.3216170	1.6588806	3.1752045
O	-2.7067002	0.7754023	1.3932608
H	-2.7308471	0.4652987	0.4480560
H	-3.5009240	1.3032264	1.5028329
O	-1.1377996	1.7945513	-2.7312367
H	-0.5976427	1.0771108	-3.1639343
H	-1.4875382	2.3267856	-3.4488284
O	0.8879045	2.4798057	-0.8605327
H	1.6269580	1.9619114	-1.2190966
H	0.1947875	2.4002156	-1.5368202
O	-0.0061357	1.4200181	1.3914036
H	-0.9772884	1.4368710	1.3225887
H	0.3428632	1.8481778	0.5641329
O	3.9037573	-2.1001795	-1.7937070
H	3.0395235	-2.1692381	-1.3611368
H	3.8552442	-2.7227649	-2.5210180
O	-2.5786835	-0.0069925	-1.1230523
H	-1.9967495	-0.7655390	-1.3166670
H	-2.2205806	0.6960913	-1.6932484
H	1.2427156	0.0620371	-3.2586044
O	0.3678247	-0.1772021	-3.6061249
H	0.0995139	-0.9093067	-3.0181544

Table 93: Cartesian coordinates (in Angstrom) of the optimized gw10-rb-4 structure, which corresponds to the Gly•$(H_2O)_{10}$ cluster after removing the exo bond.

40
Energy=-1047.3843828507

O	2.9934533	0.5368021	-1.5107694
H	3.9510976	0.5743589	-1.4775260
H	2.7302347	-0.2452529	-0.9627929
O	-1.5068317	-1.1085344	3.9142287
H	-2.0537075	-0.7609802	3.1936898
H	-1.1352272	-0.3094534	4.3248113
C	0.8365545	-1.7998482	-0.2029425
O	2.0042651	-1.3889559	0.0068219
O	0.2288768	-1.9447874	-1.2917091
H	0.5698321	-0.4246346	1.9936997
C	0.0511100	-2.1818106	1.0545165
N	0.6065602	-1.4472966	2.2131926
H	0.0051098	-1.5685762	3.0481766
H	1.5782902	-1.7029791	2.3549854
H	0.1300279	-3.2514361	1.2326187
H	-0.9966577	-1.9182992	0.9616355
O	0.1078711	1.0971775	4.4546321
H	0.1546596	1.8806815	5.0042372
H	0.1712813	1.4109850	3.5346450
O	-2.5426687	0.1994340	1.4932932
H	-2.4581878	-0.0939237	0.5446605
H	-3.3971962	0.6338311	1.5435743
O	-0.7911558	1.4805706	-2.4383099
H	-0.1148813	0.8233539	-2.7178282
H	-1.0861657	1.8130195	-3.2959601
O	1.0318333	2.3098981	-0.4482415
H	1.8003443	1.8259462	-0.7932531
H	0.3758981	2.2476964	-1.1624643
O	0.0445846	1.1782906	1.7305477
H	-0.9096416	1.0719146	1.5674627
H	0.4211345	1.6322680	0.9296367
O	-0.4366089	1.1217966	-5.2621259
H	0.1359335	0.4617807	-4.8442048
H	-0.8372438	0.6654949	-6.0030337
O	-2.1434239	-0.5071825	-1.0101984
H	-1.4355848	-1.1612498	-1.1620732
H	-1.8413262	0.2588420	-1.5324129
H	1.8890489	-0.0060043	-2.9701644
O	1.0457698	-0.3372529	-3.3179934
H	0.8227376	-1.0656843	-2.6970625

Table 94: Cartesian coordinates (in Angstrom) of the optimized gw10-rb-5 structure, which corresponds to the Gly•$(H_2O)_{10}$ cluster after removing the exo bond.

40
Energy=-1047.3841201168

O	3.1559665	0.2526936	-1.8077638
H	4.1135326	0.2091779	-1.8245019
H	2.8548171	-0.5002245	-1.2359458
O	-1.5571984	-0.9935218	3.4463140
H	-2.0668878	-0.6059802	2.7178699
H	-1.1480954	-0.2215847	3.8733721
C	0.9490284	-2.0186000	-0.4455003
O	2.0922260	-1.5609730	-0.2073005
O	0.3881590	-2.2176928	-1.5515114
H	0.7881252	-0.6746957	1.7019909
C	0.1182650	-2.3867102	0.7868837
N	0.6396707	-1.6713524	1.9746925
H	-0.0801979	-1.6437742	2.7255061
H	1.5283616	-2.0541166	2.2758816
H	0.1555389	-3.4590209	0.9599728
H	-0.9174373	-2.0938181	0.6524437
O	0.1944622	1.0776593	4.0576210
H	0.2131034	1.9038446	4.5426257
H	0.3366657	1.3121920	3.1226720
O	-2.2785669	0.2568376	0.9149520
H	-2.2911919	-0.2730478	0.0849208
H	-2.5284287	1.1399272	0.5973684
O	-0.8304268	1.3371751	-2.8388421
H	-0.1335493	0.6708579	-3.1217759
H	-1.1126333	1.7586834	-3.6547466
O	1.2785627	2.1159133	-0.9138584
H	2.0515515	1.6018279	-1.2082034
H	0.6383602	2.0021783	-1.6290191
O	0.3337624	0.9552681	1.3364922
H	-0.6064201	0.7790404	1.1157807
H	0.7117020	1.3977460	0.5408335
O	-2.1503539	2.6251704	-0.6156575
H	-1.5564158	3.3251555	-0.3353459
H	-1.6922692	2.2096315	-1.3619052
O	-2.0897470	-1.0098511	-1.4805990
H	-1.2941551	-1.5709329	-1.5694119
H	-1.9045343	-0.2682660	-2.0715153
H	1.8715480	-0.1156501	-3.1943776
O	0.9907248	-0.4088742	-3.4729312
H	0.8343755	-1.1822926	-2.8874812

Table 95: Cartesian coordinates (in Angstrom) of the optimized gw10-rb-6 structure, which corresponds to the Gly•$(H_2O)_{10}$ cluster after removing the exo bond.

40
Energy=-1047.3841200343

O	3.1435386	0.2657147	-1.8277655
H	4.1008285	0.2198135	-1.8522192
H	2.8446193	-0.4928867	-1.2623031
O	-1.5350156	-1.0287298	3.4458519
H	-2.0487425	-0.6318030	2.7253270
H	-1.1210063	-0.2626277	3.8786311
C	0.9409941	-2.0155957	-0.4751522
O	2.0868958	-1.5631802	-0.2400215
O	0.3717876	-2.2010901	-1.5792725
H	0.7983175	-0.6955596	1.6884881
C	0.1182165	-2.3957192	0.7589483
N	0.6497330	-1.6949746	1.9509366
H	-0.0645005	-1.6744096	2.7073126
H	1.5398428	-2.0829253	2.2411411
H	0.1542594	-3.4700203	0.9196284
H	-0.9177869	-2.0991738	0.6351846
O	0.2267075	1.0306871	4.0682884
H	0.2508028	1.8510951	4.5627662
H	0.3628682	1.2757536	3.1351498
O	-2.2712265	0.2520557	0.9342676
H	-2.2909963	-0.2686302	0.0985440
H	-2.5212626	1.1391862	0.6283183
O	-0.8478339	1.3710783	-2.8174588
H	-0.1546942	0.7062220	-3.1126959
H	-1.1345872	1.8026975	-3.6264514
O	1.2768408	2.1229284	-0.8992606
H	2.0466111	1.6107035	-1.2050142
H	0.6313197	2.0188243	-1.6111081
O	0.3457342	0.9395441	1.3449629
H	-0.5963911	0.7680771	1.1288703
H	0.7191828	1.3900230	0.5516867
O	-2.1484174	2.6373594	-0.5705601
H	-1.5504765	3.3323698	-0.2864182
H	-1.6968492	2.2290711	-1.3247280
O	-2.1027658	-0.9882434	-1.4764225
H	-1.3092913	-1.5502013	-1.5775433
H	-1.9203236	-0.2405824	-2.0604960
H	1.8478566	-0.0834755	-3.2087242
O	0.9644905	-0.3718695	-3.4842637
H	0.8107203	-1.1515064	-2.9064248

Table 96: Cartesian coordinates (in Angstrom) of the optimized gw10-rb-8 structure, which corresponds to the Gly•$(H_2O)_{10}$ cluster after removing the exo bond.

40
Energy=-1047.3885182164

O	3.2812184	0.1136987	-2.2277036
H	4.2371784	0.0419470	-2.2067537
H	2.9404381	-0.6105391	-1.6482397
O	-0.3114437	-1.2553723	4.1154764
H	-1.2371292	-1.2128683	3.8370544
H	-0.1318855	-0.3112414	4.2783780
C	0.8500048	-1.7878921	-0.7145864
O	2.0875722	-1.5999860	-0.5960555
O	0.1688125	-1.9159066	-1.7583725
H	0.7582492	-0.1434795	1.4539022
C	0.0901442	-1.8888514	0.6152427
N	0.8708771	-1.1674107	1.6423740
H	0.5437605	-1.3546011	2.6125667
H	1.8497995	-1.4050096	1.4770429
H	-0.0063458	-2.9338704	0.9000079
H	-0.8979642	-1.4467551	0.5432129
O	-0.3601185	1.5346132	3.8394457
H	-1.2887151	1.3522107	3.6501699
H	0.0024587	1.7741163	2.9744677
O	-2.4185298	0.9511171	0.4227971
H	-2.3026200	0.4699003	-0.4529298
H	-3.0113923	1.6820309	0.2319241
O	-0.3639044	1.4339729	-3.3785059
H	0.2129239	0.6898658	-3.7080746
H	-0.5975916	1.9458720	-4.1554897
O	1.4692032	2.0963212	-1.2877604
H	2.2040485	1.5260804	-1.5673454
H	0.8321503	2.0245357	-2.0168471
O	0.2803708	1.4178941	1.0129264
H	-0.6569952	1.3892539	0.7502281
H	0.7594141	1.7188924	0.1997886
O	-2.7047359	-0.0832164	2.9545337
H	-3.6266225	-0.2140808	3.1854441
H	-2.7136625	0.1971467	2.0184635
O	-1.9948127	-0.2391250	-1.8362866
H	-1.3424466	-0.9685021	-1.8036307
H	-1.5710486	0.4008970	-2.4360688
H	2.0567949	-0.3691678	-3.6554440
O	1.1744231	-0.6109581	-3.9740789
H	0.8681218	-1.2415326	-3.2912736

Table 97: Cartesian coordinates (in Angstrom) of the optimized gw10-rb-9 structure, which corresponds to the Gly•$(H_2O)_{10}$ cluster after removing the exo bond.

40
Energy=-1047.3845712261

O	3.1136961	-0.0275075	-2.2667257
H	4.0558372	-0.1862622	-2.3473975
H	2.7625878	-0.7539297	-1.6926967
O	-0.8752916	-0.7921404	3.7193911
H	-1.4227802	-0.3262646	3.0676993
H	-0.2957444	-0.0965572	4.0723587
C	0.7099429	-1.9168629	-0.6725089
O	1.9512839	-1.7392205	-0.6196319
O	-0.0457212	-1.9401169	-1.6752701
H	0.9729648	-0.4990113	1.5082580
C	0.0343548	-2.1437032	0.6829040
N	0.8504697	-1.5103984	1.7428383
H	0.3482147	-1.5146816	2.6519628
H	1.7717738	-1.9350906	1.7717847
H	-0.0482840	-3.2095776	0.8813936
H	-0.9568581	-1.7053947	0.7150414
O	1.2453820	1.0062794	4.0162101
H	1.5135029	1.7498242	4.5580216
H	1.2364548	1.3349721	3.0999372
O	-1.9267848	0.6737457	1.4219050
H	-1.8847947	0.3583449	0.4918778
H	-2.8290642	1.0188980	1.4532979
O	-0.5210354	1.6127798	-2.8362244
H	-0.0432846	0.8748699	-3.3097936
H	-0.8526967	2.1950896	-3.5226744
O	1.6354267	2.0485187	-1.0338006
H	2.2693485	1.4304247	-1.4352050
H	0.8965566	2.0634439	-1.6636479
O	0.7827478	1.2019217	1.3304743
H	-0.1817522	1.3285521	1.3301024
H	1.1155699	1.5589794	0.4653366
O	-4.4078173	0.6866963	0.0721684
H	-3.8072527	0.3125938	-0.5890695
H	-5.1397880	1.0487913	-0.4282960
O	-1.9928307	-0.0873924	-1.1942733
H	-1.4598563	-0.8801683	-1.4141719
H	-1.6041038	0.6007781	-1.7670625
H	1.7175858	-0.2825383	-3.5883966
O	0.7893560	-0.4357209	-3.8205689
H	0.5226844	-1.1229643	-3.1755478

Table 98: Cartesian coordinates (in Angstrom) of the optimized gw9-rb-10 structure, which corresponds to the Gly•$(H_2O)_9$ cluster after removing the exo bond.

37
Energy=-971.0467118817

O	-0.0484896	3.0752913	-0.1997762
H	-0.4942361	3.8903419	0.0359647
H	0.0931274	2.5862831	0.6435822
O	-1.0937520	-1.8153096	2.9442765
H	-0.1965576	-1.4602270	2.7802364
H	-1.6024118	-1.0099168	3.1220987
C	1.1117896	0.4310933	1.5093646
O	0.3647831	1.3945541	1.8419963
O	1.2382439	-0.6817625	2.0603737
H	1.4750591	-1.1322083	-0.5871793
C	1.9881688	0.6591493	0.2726622
N	2.3656817	-0.6634139	-0.2753515
H	2.9797715	-0.5615158	-1.0944593
H	2.7579351	-1.2245083	0.4764222
H	2.8859158	1.2079292	0.5465494
H	1.4655068	1.2129247	-0.4987380
O	-3.0786063	0.0757361	0.1480779
H	-2.8754346	0.4309782	1.0277885
H	-2.8911949	-0.8701511	0.2403796
O	-1.9077006	-2.5347699	0.5548670
H	-1.6074823	-2.3456059	1.4872106
H	-2.2890571	-3.4144023	0.5718207
O	3.1642981	0.1102754	-2.7681431
H	2.2690751	0.1294196	-3.1711198
H	3.7823174	0.1630010	-3.4979043
O	-1.1595846	0.9766098	-1.5838884
H	-1.9610585	0.7447150	-1.0663825
H	-0.8328853	1.7937908	-1.1588392
O	-2.0869123	0.8324112	2.7382356
H	-1.1573294	1.0856753	2.5199032
H	-2.3836613	1.4671224	3.3929467
O	-0.0345309	-1.4785134	-1.1534376
H	-0.6461686	-1.9828888	-0.5803679
H	-0.4529320	-0.5937829	-1.2361044
O	0.5819797	-0.0622788	-3.6076859
H	0.3523368	-0.9348997	-3.2679775
H	-0.0760041	0.4988534	-3.1674015

Table 99: Cartesian coordinates (in Angstrom) of the optimized gw9-rb-11 structure, which corresponds to the Gly•$(H_2O)_9$ cluster after removing the exo bond.

37
Energy=-971.0465680617

O	2.2219218	1.0811109	-3.4996463
H	2.3565685	1.9877439	-3.7789385
H	1.2491555	0.9494616	-3.5226737
O	-1.1015480	-0.9344423	3.5348432
H	-0.2629341	-0.5232055	3.2403371
H	-1.7108574	-0.1811397	3.5279543
C	0.7484608	0.9045921	1.3314320
O	-0.2341128	1.6846992	1.2024267
O	1.0669535	0.1933879	2.3096914
H	1.4302321	-1.1988894	-0.1513463
C	1.6917329	0.8048543	0.1263976
N	2.2352158	-0.5726512	0.1029008
H	3.0053871	-0.6598828	-0.5799608
H	2.5055658	-0.7915025	1.0621669
H	2.5115932	1.5100289	0.2398731
H	1.1856664	0.9957936	-0.8128957
O	-3.4937939	-0.2352502	0.5488886
H	-3.3565685	0.3609338	1.3025800
H	-3.1159952	-1.0748422	0.8536932
O	-1.8457881	-2.4083640	1.4869662
H	-1.5562367	-1.9171796	2.3049839
H	-2.1165145	-3.2780377	1.7874276
O	3.9847933	-0.3017468	-1.9991310
H	4.4699063	-0.9142849	-2.5540372
H	3.3946781	0.1917288	-2.6077650
O	-1.4837054	0.6535807	-1.0156111
H	-2.3250019	0.3669029	-0.5890469
H	-1.0642071	1.1997206	-0.3198654
O	-2.4565065	1.3893648	2.6587327
H	-1.6011026	1.5996879	2.2095310
H	-2.7472524	2.2084651	3.0636916
O	-0.0936188	-1.7352542	-0.5713513
H	-0.6345602	-2.1218143	0.1428077
H	-0.6049000	-0.9419878	-0.8249683
O	-0.4636604	0.8110254	-3.5231639
H	-0.8534997	0.0911063	-4.0220616
H	-0.9354669	0.8062867	-2.6648626

Table 100: Cartesian coordinates (in Angstrom) of the optimized gw9-rb-1 structure, which corresponds to the Gly•$(H_2O)_9$ cluster after removing the exo bond.

37
Energy=-971.0392853526

O	0.1007497	0.9729367	-3.6900516
H	0.0973423	1.8101277	-4.1570881
H	-0.5357998	1.0882033	-2.9582928
O	-0.7481982	-1.3222879	2.6207795
H	0.1558268	-1.1559973	2.3120927
H	-1.0703636	-0.4105757	2.7639380
C	1.3041799	0.6579107	0.6223152
O	0.5288054	1.6431925	0.6877472
O	1.6257495	-0.1471804	1.5348912
H	1.0011723	-1.4088909	-0.9870455
C	1.9561890	0.3982574	-0.7373444
N	2.0029662	-1.0655126	-0.9663248
H	2.4031561	-1.2597335	-1.8929236
H	2.4958064	-1.5048152	-0.1935326
H	2.9707062	0.7898808	-0.7364217
H	1.4003990	0.8486818	-1.5511528
O	-3.2022951	0.6407797	0.5137174
H	-2.8512752	1.0002832	1.3407929
H	-3.1279531	-0.3188688	0.6254053
O	-2.3768447	-2.1313259	0.7446308
H	-1.7654026	-1.9300899	1.5038806
H	-2.8692622	-2.9159396	0.9922617
O	1.1279118	1.2278911	4.0444529
H	1.8016242	1.9032801	4.1378317
H	1.3752043	0.7554473	3.2313029
O	-1.2699653	1.1700996	-1.3348755
H	-2.0914078	1.0741119	-0.8031518
H	-0.6329211	1.5212970	-0.6799779
O	-1.3597140	1.3876801	2.6541180
H	-0.6728764	1.5706663	1.9775506
H	-0.8788500	1.5894183	3.4683584
O	-0.5875736	-1.5292758	-1.2467607
H	-1.2134129	-1.9202474	-0.6078068
H	-0.9047374	-0.6093116	-1.3427730
O	2.2272844	-0.8007944	-3.6972683
H	2.1195678	-1.4239242	-4.4179367
H	1.4642116	-0.1953741	-3.7753386

Table 101: Cartesian coordinates (in Angstrom) of the optimized gw9-rb-2 structure, which corresponds to the Gly•$(H_2O)_9$ cluster after removing the exo bond.

37
Energy=-971.0500183277

O	0.2791047	1.4927353	-3.5062246
H	0.2222210	2.4037761	-3.7981325
H	-0.4305527	1.3929698	-2.8400553
O	-1.2779947	-1.0442207	3.0151942
H	-0.3951451	-0.7236022	2.7418778
H	-1.7819757	-0.2210363	3.0989386
C	0.8608086	0.7500380	1.0195151
O	-0.0582864	1.6089705	0.9882753
O	1.0711656	-0.1109971	1.9106962
H	1.2085287	-1.1095250	-0.7415052
C	1.8306140	0.7722582	-0.1667477
N	2.1217460	-0.6043460	-0.6393453
H	2.5404595	-0.5470249	-1.5798472
H	2.7268105	-1.0920706	0.0352645
H	2.7645002	1.2395721	0.1382832
H	1.4083430	1.3315030	-0.9944632
O	-3.5218231	0.3357536	0.0584863
H	-3.3308753	0.8141823	0.8802748
H	-3.2913717	-0.5802681	0.2776722
O	-2.2706894	-2.1462860	0.8346349
H	-1.9073858	-1.8079809	1.6969795
H	-2.6648575	-2.9982259	1.0307658
O	3.4691338	-1.3014151	1.6722848
H	2.6253493	-0.9275283	2.0050571
H	3.6589620	-2.0624375	2.2229650
O	-1.3632753	1.1236775	-1.3850045
H	-2.2566816	0.9059162	-1.0355182
H	-0.9041339	1.4673990	-0.5929585
O	-2.3326569	1.5078023	2.4001514
H	-1.4488140	1.6300711	1.9787288
H	-2.5031309	2.3149184	2.8891060
O	-0.3782584	-1.4999191	-1.0974857
H	-0.9824930	-1.8772204	-0.4319880
H	-0.7894163	-0.6428001	-1.3137950
O	2.6093759	0.0845199	-3.2808094
H	2.7039286	-0.4743087	-4.0540285
H	1.7887665	0.5951497	-3.4372424

Table 102: Cartesian coordinates (in Angstrom) of the optimized gw9-rb-3 structure, which corresponds to the Gly•$(H_2O)_9$ cluster after removing the exo bond.

37
Energy=-971.0500183372

O	-0.0759624	1.6935450	-3.4239498
H	-0.1597530	2.6196712	-3.6557340
H	-0.7142231	1.5534295	-2.6957420
O	-0.9667180	-1.2209308	3.0645381
H	-0.1158384	-0.8814393	2.7214056
H	-1.4578019	-0.4060178	3.2472382
C	0.9621941	0.6924571	0.9677341
O	0.0474170	1.5491661	1.0802120
O	1.2594198	-0.2184482	1.7812152
H	1.1237463	-1.0606503	-0.9247574
C	1.8064215	0.7864465	-0.3076988
N	2.0440951	-0.5595109	-0.8866000
H	2.3653882	-0.4462845	-1.8597769
H	2.7130246	-1.0839137	-0.3064360
H	2.7677913	1.2381692	-0.0725889
H	1.3036781	1.3913250	-1.0544048
O	-3.4965945	0.3204789	0.4372870
H	-3.2213413	0.7508977	1.2617342
H	-3.2475063	-0.6060163	0.5780324
O	-2.1793756	-2.1982629	0.9362844
H	-1.7290957	-1.9092758	1.7752133
H	-2.5523878	-3.0621110	1.1214098
O	3.6178085	-1.3844208	1.2318046
H	3.8626224	-2.1738791	1.7168358
H	2.8131389	-1.0335443	1.6698720
O	-1.4949149	1.1980731	-1.1711601
H	-2.3482822	0.9571543	-0.7451958
H	-0.9561468	1.4968943	-0.4117451
O	-2.0712461	1.3591700	2.7089650
H	-1.2349213	1.5082470	2.2069435
H	-2.1897178	2.1374526	3.2565319
O	-0.4922882	-1.4343225	-1.1378501
H	-1.0263289	-1.8515615	-0.4370746
H	-0.9212515	-0.5675412	-1.2610658
O	2.2611523	0.2816223	-3.5203022
H	2.2735956	-0.2337382	-4.3286015
H	1.4302020	0.7976692	-3.5625733

Table 103: Cartesian coordinates (in Angstrom) of the optimized gw9-rb-4 structure, which corresponds to the Gly•$(H_2O)_9$ cluster after removing the exo bond.

37
Energy=-971.0395914579

O	0.3992704	1.1188520	-3.6664219
H	0.3646487	1.9751476	-4.0961248
H	-0.3174423	1.1393096	-3.0029994
O	-0.8727911	-1.3758230	2.5430451
H	0.0238180	-1.1005983	2.2884783
H	-1.3114095	-0.5083432	2.6465763
C	1.1637174	0.7621512	0.7483560
O	0.2808978	1.6538403	0.7525982
O	1.4661033	-0.0445984	1.6666144
H	1.2652838	-1.2521571	-0.9263375
C	1.9909062	0.6333652	-0.5318032
N	2.2176213	-0.8068015	-0.8018034
H	2.7203362	-0.9192711	-1.6917961
H	2.6822042	-1.2248653	-0.0006046
H	2.9510497	1.1259597	-0.3981045
H	1.4858682	1.0608628	-1.3899818
O	-3.2854441	0.3394214	0.1525757
H	-3.0713911	0.7302353	1.0115577
H	-3.1141398	-0.6060391	0.2770439
O	-2.1845864	-2.3272699	0.4870491
H	-1.6926502	-2.0736660	1.3141234
H	-2.6172509	-3.1624853	0.6732030
O	0.5748885	1.2385397	4.1455925
H	0.9502332	0.8303510	3.3479291
H	0.7634498	0.6033525	4.8387772
O	-1.2231057	1.0837345	-1.4707039
H	-2.0867087	0.9011230	-1.0383926
H	-0.6999353	1.4727510	-0.7404363
O	-1.7863910	1.2546957	2.4883382
H	-1.0427521	1.4902418	1.8923887
H	-1.4201437	1.4902294	3.3510169
O	-0.2767997	-1.5312326	-1.3264127
H	-0.9145317	-1.9869428	-0.7449835
H	-0.6768918	-0.6480025	-1.4538256
O	2.6884244	-0.4205623	-3.4842717
H	2.7273235	-1.0220132	-4.2299010
H	1.8783204	0.1065080	-3.6303592

Table 104: Cartesian coordinates (in Angstrom) of the optimized gw9-rb-5 structure, which corresponds to the Gly•$(H_2O)_9$ cluster after removing the exo bond.

37
Energy=-971.0380239921

O	0.6149455	1.4454842	-3.3441909
H	0.5430734	2.3653068	-3.6047865
H	-0.0375652	1.3359675	-2.6255533
O	-0.2407896	-1.7189590	2.8818650
H	0.5895995	-1.3092366	2.5580984
H	-0.7503862	-0.9541521	3.1837377
C	1.5926600	0.4482600	0.9459052
O	0.7308377	1.3441105	1.1561113
O	1.8910493	-0.5456601	1.6431630
H	1.7288740	-1.2524397	-1.0049189
C	2.3880721	0.5845485	-0.3574587
N	2.6651089	-0.7799826	-0.8679248
H	3.1284587	-0.7316049	-1.7831215
H	3.1787988	-1.2960935	-0.1590886
H	3.3295428	1.0941665	-0.1673953
H	1.8384867	1.1246528	-1.1193787
O	-2.7611184	-0.0796241	0.5869022
H	-2.2325803	0.1461276	1.3844385
H	-2.6463355	-1.0389608	0.5176798
O	-1.4392093	-2.6282520	0.7256458
H	-0.9910226	-2.3489898	1.5727631
H	-1.6877561	-3.5455963	0.8539668
O	-3.7885061	2.2008060	1.9655318
H	-4.6686549	2.3240922	2.3238125
H	-3.8574768	1.4233908	1.3950428
O	-0.8401121	1.0256000	-1.0701862
H	-1.6775803	0.7349706	-0.6572683
H	-0.3065878	1.3157259	-0.2991745
O	-1.3920284	0.8521607	2.7534193
H	-0.5752312	1.1769063	2.3152905
H	-2.0061997	1.5949368	2.8188544
O	0.1616506	-1.5984761	-1.2825613
H	-0.3478600	-2.0892172	-0.6082853
H	-0.2684033	-0.7233511	-1.2999196
O	2.9814360	0.0243011	-3.4906700
H	3.0088806	-0.4485024	-4.3241708
H	2.1439292	0.5275833	-3.5161748

Table 105: Cartesian coordinates (in Angstrom) of the optimized gw9-rb-6 structure, which corresponds to the Gly•$(H_2O)_9$ cluster after removing the exo bond.

37
Energy=-971.0345748445

O	0.7334169	1.2673716	-3.2966105
H	0.7094491	2.1809596	-3.5864765
H	0.0360182	1.1995790	-2.6163102
O	-0.6024036	-1.5450491	2.9548675
H	0.2921940	-1.2751915	2.6551619
H	-1.0310442	-0.6944261	3.1242746
C	1.4991408	0.2812232	1.0367871
O	0.6919622	1.2402901	1.1953918
O	1.7045789	-0.7069547	1.7716263
H	1.5867959	-1.4794519	-0.8592809
C	2.3382367	0.3344148	-0.2423149
N	2.5459228	-1.0545614	-0.7178764
H	3.0214144	-1.0465540	-1.6296043
H	3.0270309	-1.5856413	0.0020127
H	3.3029467	0.7913659	-0.0353516
H	1.8451347	0.8900682	-1.0313710
O	-2.9413466	0.0703226	0.4835425
H	-2.6392890	0.3961021	1.3427040
H	-2.7678812	-0.8834154	0.5298876
O	-1.7673563	-2.5165994	0.8091739
H	-1.3343448	-2.2332693	1.6606286
H	-2.1581919	-3.3750125	0.9832206
O	-3.0546171	3.1407782	0.9329859
H	-2.5030876	2.6202991	1.5265435
H	-3.5690856	2.4717019	0.4755846
O	-0.8323891	0.9139178	-1.0898936
H	-1.7127971	0.7383581	-0.7006200
H	-0.3194922	1.2351674	-0.3209958
O	-1.4525497	1.2168067	2.7101699
H	-0.5678038	1.2752308	2.2596246
H	-1.3949280	1.7710598	3.4919038
O	0.0162714	-1.7440377	-1.1736946
H	-0.5525338	-2.1769232	-0.5096541
H	-0.3594940	-0.8447180	-1.2373073
O	2.9911959	-0.3169092	-3.3340282
H	3.0237559	-0.8026247	-4.1599274
H	2.1951700	0.2463226	-3.4047742

Table 106: Cartesian coordinates (in Angstrom) of the optimized gw9-rb-7 structure, which corresponds to the Gly•$(H_2O)_9$ cluster after removing the exo bond.

37
Energy=-971.0344418327

O	0.6269319	1.1871910	-3.2536683
H	0.5778335	2.0818186	-3.5950641
H	-0.0728251	1.1371506	-2.5745595
O	-0.6363466	-1.5279870	3.0606445
H	0.2509258	-1.2438050	2.7525425
H	-1.0989963	-0.6886155	3.1934626
C	1.4072466	0.2542298	1.0680238
O	0.5560764	1.1771967	1.2101473
O	1.6502045	-0.7147993	1.8162073
H	1.5336803	-1.4866359	-0.8338763
C	2.2522717	0.3288979	-0.2062819
N	2.4860914	-1.0564345	-0.6807943
H	2.9726368	-1.0446353	-1.5865808
H	2.9626309	-1.5811561	0.0471577
H	3.2076462	0.8017572	0.0075459
H	1.7531222	0.8761348	-0.9975590
O	-2.9978788	-0.0619035	0.4238023
H	-2.8514024	0.3781774	1.2716026
H	-2.7484348	-0.9851638	0.5908971
O	-1.7214392	-2.5547565	0.9094075
H	-1.3123582	-2.2533025	1.7680244
H	-2.0978428	-3.4202342	1.0799465
O	-2.2919551	3.4094418	0.6070543
H	-2.1566750	2.7385080	1.2836639
H	-2.0181422	2.9641000	-0.1985755
O	-0.9841518	0.9659611	-1.0502013
H	-1.8172293	0.6357010	-0.6389533
H	-0.4277595	1.1847529	-0.2723316
O	-1.6186751	1.1904091	2.6993434
H	-0.7254420	1.2342525	2.2708186
H	-1.5888202	1.8033467	3.4378502
O	-0.0509279	-1.7449067	-1.1362902
H	-0.5962015	-2.1662955	-0.4435366
H	-0.4522337	-0.8645421	-1.2389716
O	2.9291156	-0.3356884	-3.2969310
H	2.9841129	-0.8183866	-4.1233781
H	2.1152108	0.2002214	-3.3705888

Table 107: Cartesian coordinates (in Angstrom) of the optimized gw9-rb-8 structure, which corresponds to the Gly•$(H_2O)_9$ cluster after removing the exo bond.

37
Energy=-971.0392333239

O	0.4134216	1.5540652	-2.9744974
H	0.0633559	2.0937143	-3.6864929
H	-0.3594183	1.3035853	-2.4256070
O	-0.8936410	-1.4747074	3.2417737
H	-0.0158819	-1.1931846	2.9124237
H	-1.3470326	-0.6294364	3.3766571
C	1.1617667	0.2876734	1.1215118
O	0.3403345	1.2516887	1.2137269
O	1.3614285	-0.6452116	1.9212666
H	1.2796628	-1.5967198	-0.6496379
C	2.0088083	0.2615304	-0.1518719
N	2.2352664	-1.1542082	-0.5283459
H	2.7118174	-1.1939509	-1.4331715
H	2.7241005	-1.6331490	0.2220931
H	2.9615534	0.7561773	0.0175749
H	1.5144278	0.7495651	-0.9799691
O	-3.2997133	0.0239928	0.5367740
H	-3.0165971	0.4834414	1.3434384
H	-3.0740781	-0.9021807	0.7156541
O	-2.0322126	-2.5038632	1.1106335
H	-1.6108654	-2.1880407	1.9577486
H	-2.4334335	-3.3503685	1.3167238
O	1.4026265	3.3688123	-0.5656200
H	0.9658653	2.8304623	0.1078061
H	1.0939560	2.9916040	-1.3951067
O	-1.2255040	0.7423196	-1.0172342
H	-2.1062261	0.5534924	-0.6149657
H	-0.7106262	1.0620885	-0.2494819
O	-1.8600698	1.1460654	2.7533025
H	-0.9970009	1.2660715	2.2910215
H	-1.9870820	1.9392749	3.2773984
O	-0.2842092	-1.8914481	-0.9468106
H	-0.8424354	-2.2618893	-0.2357130
H	-0.6785505	-1.0110302	-1.0983620
O	2.4364916	-0.4105844	-3.2053978
H	2.3627995	-0.8915817	-4.0313598
H	1.7368952	0.2659298	-3.2478835

Table 108: Cartesian coordinates (in Angstrom) of the optimized gw9-rb-9 structure, which corresponds to the Gly•$(H_2O)_9$ cluster after removing the exo bond.

37
Energy=-971.0499065723

O	-0.1341130	2.0933531	-2.8144089
H	-0.5742151	2.7171022	-3.3937444
H	-0.7861637	1.8711223	-2.1218499
O	-0.8451837	-1.7026939	3.0891493
H	-0.0154021	-1.2152847	2.9114124
H	-1.4444784	-0.9889361	3.3544622
C	0.9172122	0.7592604	1.5096585
O	-0.0587279	1.5418335	1.6654014
O	1.2780274	-0.2000907	2.2268448
H	1.5018070	-0.8570304	-0.5062308
C	1.7920111	1.0000113	0.2698733
N	2.3201846	-0.3199545	-0.1453963
H	3.0405234	-0.2594461	-0.8857023
H	2.6369178	-0.7850547	0.7062944
H	2.6218946	1.6527251	0.5296754
H	1.2386717	1.4351250	-0.5557151
O	-3.4106416	-0.1478081	0.6700852
H	-3.2053657	0.1863661	1.5580821
H	-3.0438630	-1.0449377	0.6726013
O	-1.7439671	-2.5223323	0.7557517
H	-1.3890630	-2.2885670	1.6576821
H	-2.0118833	-3.4417422	0.8106325
O	3.6968246	-0.2612714	-2.4952018
H	4.3189590	0.2603771	-3.0033891
H	2.8425427	-0.2308147	-2.9856225
O	-1.4560497	1.1571463	-0.6526546
H	-2.2880257	0.7665807	-0.2965830
H	-1.0024347	1.4857361	0.1511823
O	-2.1977148	0.7778667	3.0860812
H	-1.3686378	1.1323557	2.6814145
H	-2.4587789	1.4176549	3.7509363
O	-0.1062785	-1.2188613	-1.0442106
H	-0.6203170	-1.8473868	-0.5001232
H	-0.6200977	-0.3860395	-0.9584795
O	1.1913717	-0.2598921	-3.4414218
H	0.6661544	-0.8648991	-2.9011437
H	0.7183001	0.5884267	-3.3553431

Table 109: Harmonic frequencies for the structure 1N1a, the global non–dissociated minimum of Gly•$(H_2O)_1$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol
1	-0.00	0.00000	1	-0.00	0.00000	1	-0.00	0.00000
2	0.00	0.00000	2	0.00	0.00000	2	-0.00	0.00000
3	0.00	0.00000	3	0.00	0.00000	3	-0.00	0.00000
4	0.00	0.00000	4	0.00	0.00000	4	0.00	0.00000
5	0.00	0.00000	5	0.00	0.00000	5	0.00	0.00000
6	0.00	0.00000	6	0.00	0.00000	6	0.00	0.00000
7	55.31	4.10940	7	54.20	3.95919	7	55.05	4.08992
8	72.08	2.05766	8	69.65	1.80392	8	71.94	2.04023
9	145.23	9.95358	9	140.42	9.42850	9	144.19	9.67315
10	198.76	6.33159	10	189.73	6.80173	10	198.56	6.33430
11	215.29	62.09301	11	214.85	61.50682	11	214.67	61.91404
12	264.09	83.90510	12	262.37	76.36771	12	263.99	81.59041
13	294.08	104.24123	13	285.29	101.88093	13	292.20	105.74262
14	368.95	63.78736	14	366.10	66.42023	14	368.87	64.07673
15	495.67	17.45069	15	481.76	16.78996	15	491.85	16.99599
16	562.28	2.13895	16	558.35	1.94336	16	562.21	2.15038
17	648.18	116.55496	17	635.89	50.49771	17	648.03	115.06263
18	675.18	95.31123	18	662.95	164.16715	18	675.11	96.63829
19	861.73	98.18241	19	845.39	69.48126	19	857.67	109.64925
20	913.24	107.81462	20	910.26	113.88925	20	913.14	108.14823
21	927.12	11.53579	21	925.24	4.08080	21	927.11	11.47080
22	951.43	105.62948	22	945.99	131.86634	22	945.20	94.64764
23	1167.27	26.06848	23	1164.86	38.53901	23	1156.23	22.27540
24	1192.64	0.92265	24	1192.18	0.81846	24	1192.00	0.94656
25	1252.25	240.83268	25	1235.01	227.00390	25	1251.78	242.03018
26	1382.45	15.77600	26	1376.62	7.49199	26	1382.21	16.32969
27	1395.83	0.13953	27	1395.81	0.14751	27	1391.39	0.15612
28	1466.53	15.24120	28	1461.87	23.30340	28	1466.48	15.30382
29	1472.04	31.50949	29	1469.20	22.77957	29	1472.04	31.55875
30	1646.00	110.73727	30	1638.65	119.82443	30	1646.00	110.66101
31	1676.73	17.11024	31	1676.62	15.42225	31	1673.01	17.17410
32	1781.14	225.32102	32	1752.97	208.32443	32	1781.11	224.89829
33	3103.04	13.62309	33	3103.03	13.60040	33	3103.03	13.62061
34	3151.56	3.68295	34	3151.56	3.68329	34	3151.55	3.68542
35	3398.51	640.03175	35	3387.51	633.06031	35	3398.51	640.07227
36	3545.43	3.60893	36	3545.43	3.62207	36	3540.34	3.43829
37	3630.59	8.01561	37	3630.59	8.01523	37	3620.71	7.82874
38	3675.13	335.73127	38	3665.18	336.79787	38	3675.13	335.74179
39	3922.68	112.23980	39	3908.83	105.63331	39	3922.68	112.24088

Table 110: Harmonic frequencies for the structure 2N1a, the global non–dissociated minimum of Gly•$(H_2O)_2$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol
1	-0.00	0.00000	1	-0.00	0.00000	1	0.00	0.00000
2	-0.00	0.00000	2	0.00	0.00000	2	0.00	0.00000
3	-0.00	0.00000	3	0.00	0.00000	3	0.00	0.00000
4	0.00	0.00000	4	0.00	0.00000	4	0.00	0.00000
5	0.00	0.00000	5	0.00	0.00000	5	0.00	0.00000
6	0.00	0.00000	6	0.00	0.00000	6	0.00	0.00000
7	40.12	1.22304	7	38.65	1.14145	7	40.07	1.22253
8	52.81	3.49368	8	51.33	3.25989	8	52.49	3.43377
9	72.10	0.82151	9	69.85	0.81084	9	72.00	0.85168
10	100.72	1.07547	10	96.71	1.01821	10	100.14	1.06020
11	160.46	5.95291	11	153.90	5.55941	11	159.74	5.82504
12	208.64	16.49396	12	199.61	15.18192	12	208.36	16.41489
13	216.48	61.85451	13	215.97	60.77960	13	215.87	61.55588
14	234.92	111.51399	14	233.90	102.73265	14	234.91	111.62704
15	266.21	38.74854	15	253.60	46.17502	15	266.12	38.82976
16	307.62	8.17402	16	299.07	20.48560	16	305.93	12.04041
17	320.59	135.44172	17	316.87	114.72990	17	320.15	130.19844
18	387.53	28.21876	18	385.87	31.70200	18	387.51	28.47119
19	460.70	81.00544	19	457.60	74.96703	19	460.29	78.95925
20	519.63	26.89192	20	505.38	33.19982	20	516.39	29.51644
21	569.06	0.74466	21	564.64	0.59963	21	568.98	0.75382
22	661.07	32.69699	22	642.02	17.77609	22	660.87	32.31789
23	697.94	130.72149	23	693.83	141.95822	23	697.94	130.73802
24	864.11	77.43651	24	849.23	65.60404	24	860.02	92.58713
25	910.60	187.33455	25	907.79	161.26793	25	909.58	187.35732
26	926.63	2.47895	26	925.19	2.81213	26	926.63	2.44215
27	955.99	56.63122	27	949.10	88.99689	27	950.77	41.37047
28	1020.52	108.20123	28	1017.39	107.06035	28	1020.51	108.15830
29	1168.51	16.22092	29	1166.93	23.00574	29	1157.38	14.35807
30	1192.12	0.69975	30	1191.69	0.59792	30	1191.48	0.71853
31	1277.01	260.96986	31	1258.33	268.22986	31	1276.67	260.08584
32	1387.41	49.47356	32	1381.23	31.27713	32	1387.19	50.61352
33	1395.69	0.14425	33	1395.67	0.14422	33	1391.24	0.19266
34	1468.07	16.57199	34	1467.84	17.52888	34	1468.05	16.57062
35	1489.28	8.30239	35	1483.20	7.60723	35	1489.26	8.32935
36	1661.65	72.70825	36	1655.14	71.81421	36	1661.65	72.73837
37	1676.26	4.88758	37	1673.30	47.73022	37	1672.64	8.53172
38	1681.54	76.30100	38	1677.00	50.55513	38	1681.45	72.75955
39	1767.12	284.45864	39	1738.83	252.30897	39	1767.09	283.86233
40	3103.36	25.67043	40	3103.28	32.84965	40	3103.36	25.67508
41	3145.97	1302.51535	41	3135.03	1283.61878	41	3145.97	1302.61790
42	3152.10	4.01090	42	3152.10	3.99860	42	3152.09	4.01324
43	3484.46	613.64616	43	3473.90	612.01908	43	3484.46	613.68285
44	3545.42	2.01513	44	3545.42	2.02623	44	3540.33	1.88124
45	3603.35	828.78122	45	3593.06	830.09367	45	3603.35	828.74307
46	3630.78	7.34780	46	3630.78	7.34737	46	3620.90	7.16901

Continued on next page...

Table 110: Harmonic frequencies for the structure 2N1a, the global non–dissociated minimum of Gly•$(H_2O)_2$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number	IR intensity	mode	wave number	IR intensity	mode	wave number	IR intensity
	cm^{-1}	km/mol		cm^{-1}	km/mol		cm^{-1}	km/mol
47	3917.52	95.48012	47	3904.51	90.08934	47	3917.52	95.48016
48	3925.75	108.81478	48	3912.42	102.10554	48	3925.75	108.81518

Table 111: Harmonic frequencies for the structure 2Za, the global zwitterionic minimum of Gly•$(H_2O)_2$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number	IR intensity	mode	wave number	IR intensity	mode	wave number	IR intensity
	cm^{-1}	km/mol		cm^{-1}	km/mol		cm^{-1}	km/mol
1	-0.00	0.00000	1	-0.00	0.00000	1	-0.00	0.00000
2	-0.00	0.00000	2	-0.00	0.00000	2	-0.00	0.00000
3	-0.00	0.00000	3	0.00	0.00000	3	-0.00	0.00000
4	0.00	0.00000	4	0.00	0.00000	4	-0.00	0.00000
5	0.00	0.00000	5	0.00	0.00000	5	0.00	0.00000
6	0.00	0.00000	6	0.00	0.00000	6	0.00	0.00000
7	33.25	14.08155	7	31.71	12.83445	7	33.18	13.98760
8	54.56	1.19273	8	52.26	1.13913	8	54.51	1.16167
9	92.29	5.55381	9	88.91	5.60971	9	91.94	5.37780
10	118.52	29.56210	10	116.47	27.68523	10	118.17	29.56725
11	186.00	52.19751	11	180.14	45.78765	11	185.65	51.67693
12	195.06	101.95052	12	192.66	99.43407	12	194.65	102.40890
13	238.60	38.73348	13	227.29	34.70153	13	238.50	38.75143
14	269.33	95.57805	14	257.98	99.58539	14	268.63	90.20714
15	322.11	202.02509	15	315.86	157.16429	15	319.35	152.06022
16	324.05	6.50784	16	321.87	42.61863	16	323.57	57.41700
17	417.26	20.27080	17	416.05	21.64317	17	417.17	20.02771
18	469.79	80.00037	18	467.18	90.02869	18	468.94	80.89566
19	511.18	9.47323	19	499.91	14.34952	19	508.45	11.61951
20	552.07	105.98531	20	548.26	101.38457	20	549.54	99.77748
21	579.15	28.51699	21	573.39	23.68621	21	578.85	25.52460
22	707.90	10.27066	22	687.12	8.97539	22	706.74	11.29626
23	766.72	247.50980	23	764.17	242.63737	23	766.64	248.31632
24	877.96	61.83961	24	853.87	44.53439	24	877.84	63.42962
25	893.59	55.51508	25	890.55	64.17317	25	893.56	55.31573
26	945.89	20.70955	26	943.69	19.72458	26	945.40	20.37592
27	1025.23	1.48354	27	1024.51	1.51002	27	1016.23	3.65576
28	1093.97	230.70375	28	1092.30	235.87945	28	1087.06	236.67127
29	1116.68	16.64534	29	1115.71	16.12059	29	1115.36	18.42179
30	1201.83	221.92380	30	1192.57	207.39369	30	1197.35	221.73001
31	1309.18	32.62029	31	1304.54	30.71790	31	1305.87	32.73878
32	1333.86	11.29620	32	1333.62	11.24350	32	1330.12	13.89107
33	1368.87	300.63977	33	1351.42	317.44405	33	1367.85	298.60239

Continued on next page...

Table 111: Harmonic frequencies for the structure 2Za, the global zwitterionic minimum of Gly•$(H_2O)_2$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number	IR intensity	mode	wave number	IR intensity	mode	wave number	IR intensity
	cm^{-1}	km/mol		cm^{-1}	km/mol		cm^{-1}	km/mol
34	1488.80	13.06415	34	1488.73	13.92191	34	1488.62	13.13405
35	1604.29	25.84811	35	1604.00	26.28302	35	1601.67	23.89800
36	1674.80	38.16714	36	1668.48	41.52366	36	1674.58	35.31088
37	1694.13	107.32325	37	1690.44	95.13795	37	1693.07	112.20665
38	1711.50	11.76941	38	1708.38	20.88331	38	1710.76	9.84270
39	1793.07	309.93616	39	1764.93	285.89989	39	1793.07	310.05676
40	2465.43	476.94726	40	2465.07	476.56396	40	2461.05	474.79684
41	3149.80	7.49351	41	3149.79	7.47128	41	3149.77	7.90119
42	3227.48	5.61820	42	3227.47	5.86890	42	3227.40	9.18352
43	3250.56	382.56320	43	3249.72	375.54469	43	3244.49	384.44080
44	3385.28	824.21853	44	3375.49	828.93274	44	3384.82	819.21461
45	3534.37	572.08217	45	3523.88	570.06072	45	3534.36	572.03854
46	3614.10	66.23884	46	3614.10	66.72890	46	3605.45	63.32670
47	3894.71	77.29206	47	3881.93	73.54757	47	3894.71	77.29460
48	3924.10	82.06771	48	3911.21	77.58187	48	3924.09	82.11229

Table 112: Harmonic frequencies for the structure 3N6a, the global non–dissociated minimum of Gly•$(H_2O)_3$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number	IR intensity	mode	wave number	IR intensity	mode	wave number	IR intensity
	cm^{-1}	km/mol		cm^{-1}	km/mol		cm^{-1}	km/mol
1	-0.00	0.00000	1	-0.00	0.00000	1	-0.00	0.00000
2	-0.00	0.00000	2	-0.00	0.00000	2	0.00	0.00000
3	-0.00	0.00000	3	0.00	0.00000	3	0.00	0.00000
4	-0.00	0.00000	4	0.00	0.00000	4	0.00	0.00000
5	0.00	0.00000	5	0.00	0.00000	5	0.00	0.00000
6	0.00	0.00000	6	0.00	0.00000	6	0.00	0.00000
7	41.14	1.66559	7	39.32	1.54119	7	41.11	1.65198
8	49.09	8.54258	8	46.84	7.55826	8	48.98	8.56577
9	68.76	0.39589	9	66.25	0.45173	9	68.62	0.38039
10	81.88	2.01789	10	78.43	1.96332	10	81.54	1.93265
11	88.47	6.74386	11	85.00	6.21763	11	88.40	6.73652
12	118.76	7.56241	12	115.33	7.07062	12	118.59	7.50231
13	171.81	3.65624	13	165.05	3.65738	13	171.29	3.24109
14	180.12	70.50739	14	178.40	67.82504	14	179.95	71.28936
15	227.66	20.40776	15	221.26	12.07512	15	226.45	19.92595
16	236.78	39.99141	16	227.16	41.66333	16	236.02	38.26558
17	250.39	170.84905	17	247.08	174.99966	17	250.33	171.21722
18	276.05	14.72164	18	264.70	0.82424	18	274.96	20.06530
19	282.21	55.47796	19	275.07	64.23277	19	281.47	51.07810
20	351.22	19.95246	20	348.29	12.67443	20	349.34	15.42234

Continued on next page...

Table 112: Harmonic frequencies for the structure 3N6a, the global non–dissociated minimum of Gly•$(H_2O)_3$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol
21	374.36	42.80625	21	371.23	52.56229	21	373.61	47.25774
22	445.35	69.14636	22	440.85	65.77415	22	444.95	69.37784
23	488.15	35.49456	23	478.61	23.99761	23	486.45	32.06511
24	520.21	30.02153	24	516.29	42.59929	24	518.76	33.71713
25	530.66	24.91605	25	528.31	24.37566	25	530.48	24.58750
26	586.37	0.50809	26	575.76	0.61851	26	585.95	0.46207
27	678.41	11.88590	27	662.97	10.55061	27	677.64	12.39527
28	766.41	40.44373	28	764.18	41.33827	28	766.14	39.32154
29	814.05	289.74133	29	811.74	285.98885	29	813.49	289.40385
30	875.68	64.25984	30	860.16	16.70228	30	875.00	66.50164
31	895.34	107.10736	31	888.82	145.68506	31	895.14	107.26372
32	931.85	100.97781	32	930.95	102.40681	32	928.82	102.94655
33	1057.62	27.92962	33	1056.58	27.64913	33	1052.41	25.43664
34	1104.11	13.53727	34	1102.25	17.67280	34	1094.98	9.22098
35	1119.44	78.75005	35	1116.77	78.82300	35	1119.30	81.44902
36	1193.64	25.37212	36	1190.71	33.81849	36	1192.22	23.07871
37	1281.01	66.92632	37	1272.44	135.76203	37	1278.82	59.27826
38	1309.01	147.70495	38	1298.17	70.44481	38	1306.85	155.20439
39	1425.12	21.46883	39	1420.87	11.97158	39	1424.02	22.88455
40	1505.09	28.57625	40	1499.30	49.85360	40	1504.77	28.76259
41	1509.19	38.61140	41	1508.10	19.45388	41	1509.18	38.54302
42	1619.99	78.02414	42	1619.21	84.13710	42	1616.20	76.33760
43	1676.22	29.17357	43	1669.34	26.49793	43	1676.21	29.10581
44	1699.15	27.98378	44	1693.09	27.64258	44	1699.14	27.99029
45	1713.60	47.37364	45	1707.87	46.00943	45	1713.59	47.11940
46	1787.86	240.59630	46	1758.56	229.25621	46	1787.82	241.26794
47	3060.17	829.16191	47	3050.82	1068.02816	47	3060.17	828.98751
48	3066.05	329.83111	48	3065.14	83.63189	48	3066.05	330.00545
49	3160.49	4.40721	49	3160.49	4.33866	49	3160.48	4.41089
50	3367.99	1009.46582	50	3357.39	1003.86340	50	3367.97	1009.22024
51	3492.23	963.13154	51	3481.73	958.90739	51	3492.22	963.16924
52	3529.43	8.28833	52	3529.37	8.25043	52	3524.34	8.44364
53	3559.97	285.32682	53	3549.47	286.29976	53	3559.97	285.31842
54	3633.92	21.24309	54	3633.92	21.19431	54	3623.96	20.82275
55	3879.09	79.40387	55	3866.45	75.39184	55	3879.09	79.40233
56	3912.87	80.72551	56	3900.10	76.53528	56	3912.87	80.73110
57	3919.99	80.88319	57	3906.96	76.46190	57	3919.99	80.88512

Table 113: Harmonic frequencies for the structure 3Za, the global zwitterionic minimum of Gly•$(H_2O)_3$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol
1	0.00	0.00000	1	-0.00	0.00000	1	0.00	0.00000
2	0.00	0.00000	2	-0.00	0.00000	2	0.00	0.00000
3	0.00	0.00000	3	-0.00	0.00000	3	0.00	0.00000
4	0.00	0.00000	4	-0.00	0.00000	4	0.00	0.00000
5	0.00	0.00000	5	0.00	0.00000	5	0.00	0.00000
6	0.00	0.00000	6	0.00	0.00000	6	0.00	0.00000
7	42.62	19.71549	7	40.82	18.11869	7	42.49	19.55638
8	68.86	2.68856	8	65.55	2.33370	8	68.80	2.67053
9	108.19	4.90806	9	103.37	4.46436	9	107.81	4.84466
10	111.33	13.71560	10	106.74	12.97409	10	110.96	13.43186
11	152.44	1.48328	11	150.20	1.69902	11	151.86	1.31554
12	204.73	30.62869	12	196.80	16.13395	12	204.65	30.59188
13	212.21	1.24623	13	202.41	1.00726	13	212.10	1.30779
14	225.76	59.42063	14	219.02	33.84106	14	225.73	59.65958
15	238.05	60.52640	15	227.95	70.37282	15	238.01	60.61946
16	244.29	43.53432	16	234.57	72.74193	16	244.25	43.25864
17	272.65	70.46494	17	269.38	67.82872	17	272.43	71.13531
18	299.75	66.67313	18	292.32	61.42835	18	298.22	65.02405
19	364.42	102.53704	19	355.96	94.10307	19	360.70	98.40333
20	418.62	24.86524	20	417.20	29.47178	20	418.26	25.69005
21	475.70	51.07141	21	469.69	45.27066	21	474.67	49.71570
22	482.70	15.98482	22	477.84	8.35379	22	479.86	15.94005
23	507.24	63.53437	23	501.04	82.87810	23	506.37	64.35758
24	603.24	15.93709	24	590.98	17.73234	24	602.68	16.28842
25	604.99	10.83764	25	603.97	8.18132	25	604.86	9.53088
26	716.95	14.52063	26	704.45	14.59923	26	716.03	14.67769
27	749.59	87.51142	27	747.12	83.62298	27	749.59	87.38853
28	768.39	278.59196	28	766.58	275.39898	28	768.30	277.73662
29	858.72	62.05028	29	850.91	30.54147	29	858.45	61.62136
30	878.11	83.49871	30	862.47	95.12021	30	877.65	86.23043
31	941.68	154.81935	31	937.19	161.72444	31	941.51	154.47064
32	970.61	4.80617	32	968.27	4.49951	32	970.13	4.23172
33	1019.31	8.57117	33	1018.16	9.96406	33	1009.59	10.58696
34	1132.17	23.47789	34	1131.53	24.83194	34	1128.21	28.54925
35	1143.48	23.38932	35	1142.41	24.28396	35	1141.04	20.46854
36	1329.26	24.27103	36	1314.65	66.60971	36	1325.41	21.77800
37	1346.28	39.55184	37	1340.03	42.88336	37	1342.68	39.39859
38	1384.29	107.62346	38	1371.42	57.30333	38	1383.31	109.41197
39	1477.03	233.72239	39	1474.60	244.84395	39	1472.12	239.43283
40	1504.89	35.10500	40	1504.81	35.11240	40	1504.67	31.72143
41	1587.11	36.47228	41	1586.16	37.15944	41	1585.96	35.67754
42	1656.82	95.92575	42	1647.95	124.72812	42	1656.82	95.95483
43	1676.94	194.46466	43	1670.13	197.78428	43	1676.91	194.99947
44	1714.63	21.37972	44	1708.64	22.57173	44	1714.53	21.88458
45	1732.40	109.29111	45	1721.41	164.89110	45	1731.15	101.99097
46	1759.27	243.36581	46	1748.20	116.08428	46	1758.90	249.85773

Continued on next page...

Table 113: Harmonic frequencies for the structure 3Za, the global zwitterionic minimum of Gly•$(H_2O)_3$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number	IR intensity	mode	wave number	IR intensity	mode	wave number	IR intensity
	cm^{-1}	km/mol		cm^{-1}	km/mol		cm^{-1}	km/mol
47	2699.90	1047.02716	47	2699.82	1045.62004	47	2693.26	1047.31041
48	3138.67	3.79296	48	3138.67	3.78419	48	3138.65	3.88995
49	3221.04	2.39551	49	3221.04	2.40815	49	3220.97	2.87339
50	3272.50	112.53644	50	3272.43	110.68368	50	3266.54	114.03521
51	3404.86	426.80070	51	3393.95	418.43483	51	3404.85	426.35174
52	3469.34	546.35461	52	3459.36	559.89829	52	3469.26	543.99595
53	3530.59	593.17937	53	3521.17	603.72187	53	3530.58	594.19476
54	3580.34	762.36382	54	3566.89	745.25026	54	3580.22	733.90305
55	3593.54	61.70804	55	3593.50	58.15006	55	3585.09	87.42770
56	3917.90	72.59400	56	3904.92	69.31639	56	3917.90	72.59814
57	3921.64	105.04114	57	3908.69	97.93966	57	3921.64	105.03745

Table 114: Harmonic frequencies for the structure 4N6a, the global non–dissociated minimum of Gly•$(H_2O)_4$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number	IR intensity	mode	wave number	IR intensity	mode	wave number	IR intensity
	cm^{-1}	km/mol		cm^{-1}	km/mol		cm^{-1}	km/mol
1	-0.00	0.00000	1	-0.00	0.00000	1	-0.00	0.00000
2	0.00	0.00000	2	-0.00	0.00000	2	-0.00	0.00000
3	0.00	0.00000	3	0.00	0.00000	3	-0.00	0.00000
4	0.00	0.00000	4	0.00	0.00000	4	-0.00	0.00000
5	0.00	0.00000	5	0.00	0.00000	5	0.00	0.00000
6	0.00	0.00000	6	0.00	0.00000	6	0.00	0.00000
7	31.68	1.67289	7	30.33	1.52792	7	31.65	1.67407
8	42.53	3.61067	8	40.51	3.32263	8	42.47	3.50802
9	44.60	1.99894	9	42.59	1.82961	9	44.48	2.03484
10	64.42	3.29800	10	61.90	2.88947	10	64.18	3.35777
11	77.17	2.18212	11	73.73	1.94168	11	76.99	2.14729
12	86.74	5.51029	12	83.35	5.04560	12	86.59	5.45833
13	116.24	4.72442	13	113.48	4.51221	13	116.12	4.71076
14	159.19	5.43857	14	151.32	4.40754	14	159.15	5.44874
15	177.59	9.66409	15	169.72	6.26224	15	177.50	9.52092
16	208.84	89.63954	16	206.00	88.47875	16	208.79	89.35292
17	217.12	99.99054	17	214.04	90.42618	17	217.06	100.22127
18	224.68	22.62161	18	216.73	35.56539	18	224.41	22.23669
19	239.66	23.43958	19	233.82	24.29903	19	236.83	21.79196
20	264.17	63.90803	20	256.35	41.23049	20	263.25	66.50913
21	288.12	49.57865	21	276.70	51.32440	21	287.75	48.46216
22	305.27	31.88481	22	292.58	43.20989	22	305.12	31.22553
23	339.35	11.75368	23	335.44	8.53279	23	336.80	10.79552
24	360.03	139.51851	24	355.67	136.84077	24	359.95	141.04397

Continued on next page...

Table 114: Harmonic frequencies for the structure 4N6a, the global non–dissociated minimum of Gly•$(H_2O)_4$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol
25	442.04	20.42246	25	440.46	22.62552	25	441.89	19.67824
26	456.42	32.44645	26	454.50	32.98750	26	456.19	32.99856
27	502.38	45.26205	27	491.19	31.26657	27	500.62	40.82919
28	536.64	49.34594	28	532.48	63.29980	28	534.98	56.03467
29	540.67	13.79987	29	538.21	12.24896	29	540.22	12.58799
30	587.71	7.31989	30	578.65	5.85184	30	587.33	7.22342
31	628.66	34.94376	31	625.75	39.33019	31	628.62	34.94404
32	669.28	13.20366	32	653.45	10.71629	32	668.53	13.51886
33	722.59	20.90404	33	721.20	20.77023	33	722.56	20.93611
34	794.56	199.48444	34	791.98	196.10260	34	794.52	199.01594
35	839.11	96.30357	35	836.41	88.92687	35	837.91	95.86698
36	891.32	10.06549	36	871.85	12.58118	36	890.99	10.39349
37	937.42	201.52362	37	934.53	196.58122	37	937.39	197.12953
38	946.54	139.30418	38	945.59	135.52647	38	943.85	147.40188
39	1057.66	27.21535	39	1056.51	28.33225	39	1052.24	23.80474
40	1112.70	7.56475	40	1110.87	10.94956	40	1103.62	6.15386
41	1181.30	82.42919	41	1178.70	82.97208	41	1181.30	82.41439
42	1203.03	19.56711	42	1200.49	27.31344	42	1201.40	17.36849
43	1281.48	25.39012	43	1278.05	77.13913	43	1278.90	21.97315
44	1317.97	225.71693	44	1300.08	175.07686	44	1316.45	228.64474
45	1423.62	37.38713	45	1419.68	24.45065	45	1422.57	39.32371
46	1503.67	11.02780	46	1503.39	10.77903	46	1503.52	10.85485
47	1512.45	37.53609	47	1506.38	38.26685	47	1512.28	37.75542
48	1621.57	90.33470	48	1620.46	101.37445	48	1617.86	88.26873
49	1690.27	43.18043	49	1684.27	41.52682	49	1690.25	42.86852
50	1696.66	25.86884	50	1690.54	25.55689	50	1696.65	25.86588
51	1705.03	77.25011	51	1698.57	101.10799	51	1705.03	77.32402
52	1720.76	133.83840	52	1713.00	144.40449	52	1720.76	133.88790
53	1770.94	211.30881	53	1744.44	155.54263	53	1770.89	212.19990
54	2916.27	1758.91035	54	2905.80	1747.54386	54	2916.27	1758.93423
55	3067.68	26.72135	55	3067.67	26.73863	55	3067.68	26.73051
56	3155.58	2.99619	56	3155.58	2.97172	56	3155.57	2.99732
57	3344.52	949.11487	57	3333.95	943.94844	57	3344.52	948.98724
58	3394.97	1129.31984	58	3384.38	1123.26521	58	3394.94	1128.87036
59	3434.61	653.50021	59	3424.12	652.91559	59	3434.61	653.78995
60	3527.03	9.83412	60	3526.97	9.40617	60	3521.89	10.16107
61	3618.89	361.79498	61	3608.49	365.39629	61	3618.86	341.44484
62	3631.68	26.63075	62	3631.68	24.27948	62	3621.83	46.44029
63	3804.65	217.30658	63	3791.94	212.20165	63	3804.65	217.29418
64	3904.28	80.02514	64	3891.60	75.96826	64	3904.28	80.02464
65	3917.75	81.02960	65	3904.86	76.18235	65	3917.75	81.03920
66	3927.02	74.47163	66	3914.10	70.62597	66	3927.02	74.47177

Table 115: Harmonic frequencies for the structure 4Za, the global zwitterionic minimum of Gly•$(H_2O)_4$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol
1	-0.00	0.00000	1	-0.00	0.00000	1	-0.00	0.00000
2	-0.00	0.00000	2	0.00	0.00000	2	-0.00	0.00000
3	0.00	0.00000	3	0.00	0.00000	3	-0.00	0.00000
4	0.00	0.00000	4	0.00	0.00000	4	-0.00	0.00000
5	0.00	0.00000	5	0.00	0.00000	5	-0.00	0.00000
6	0.00	0.00000	6	0.00	0.00000	6	0.00	0.00000
7	39.10	7.46508	7	37.24	6.77124	7	39.10	7.45966
8	55.82	11.06462	8	53.67	10.18317	8	55.60	10.97413
9	62.39	0.56597	9	59.49	0.44316	9	62.30	0.57928
10	94.21	3.07784	10	89.57	2.98581	10	94.07	3.00092
11	105.45	1.21228	11	100.61	1.05226	11	105.16	1.23974
12	129.20	3.76936	12	126.03	3.45140	12	129.17	3.76703
13	191.17	1.36419	13	183.85	1.00014	13	190.55	1.27660
14	211.29	6.04145	14	201.27	1.70778	14	211.29	6.02637
15	214.81	13.36940	15	204.28	11.73666	15	214.56	13.39588
16	224.76	38.76691	16	214.02	32.19337	16	224.55	40.18759
17	233.06	61.54839	17	226.87	48.86366	17	232.88	58.63398
18	252.79	73.26183	18	245.40	98.22967	18	252.56	73.21896
19	264.83	86.76126	19	254.94	68.90907	19	264.47	87.68123
20	283.39	35.22694	20	280.78	34.83883	20	283.04	33.87030
21	301.71	55.70950	21	299.88	54.38022	21	301.37	52.61703
22	324.66	124.05174	22	317.83	125.26602	22	320.75	123.77127
23	356.12	117.77647	23	346.82	115.99024	23	352.36	116.05329
24	415.91	28.81449	24	414.30	30.19159	24	415.88	28.49184
25	452.46	21.07797	25	443.85	13.09904	25	450.63	21.17369
26	488.19	105.94657	26	486.91	114.30058	26	488.12	106.96729
27	506.22	4.35357	27	502.85	25.76401	27	505.76	4.79715
28	513.74	125.80780	28	510.11	111.46118	28	513.23	125.98332
29	615.74	22.27975	29	601.35	21.23373	29	615.05	21.59927
30	619.01	16.22601	30	618.10	16.61069	30	619.00	16.12742
31	746.65	37.12596	31	736.76	21.64295	31	745.69	34.48872
32	756.40	97.25076	32	753.61	110.49342	32	756.27	100.12037
33	786.14	246.69199	33	784.25	243.11309	33	786.00	245.64991
34	843.82	252.12465	34	839.68	206.58393	34	843.36	250.35119
35	866.53	16.20758	35	863.52	58.20366	35	866.38	17.16476
36	889.84	110.39686	36	871.72	85.79366	36	889.28	112.37987
37	954.41	99.55125	37	948.99	113.28704	37	954.21	100.56540
38	979.71	1.45137	38	976.99	1.18859	38	979.68	1.42460
39	1029.64	2.46735	39	1026.93	4.11700	39	1019.56	2.45949
40	1157.70	24.88553	40	1157.05	26.79247	40	1152.99	26.83805
41	1169.77	28.49063	41	1167.93	30.10956	41	1169.08	28.63994
42	1352.83	24.59787	42	1335.96	54.45962	42	1350.72	21.29974
43	1379.99	26.65579	43	1375.85	24.91050	43	1375.31	28.64642
44	1422.74	93.53241	44	1410.91	57.67485	44	1421.70	95.25208
45	1500.97	5.22414	45	1500.87	6.21821	45	1500.68	5.21219
46	1589.08	120.01673	46	1588.44	119.59609	46	1583.94	121.73488

Continued on next page...

Table 115: Harmonic frequencies for the structure 4Za, the global zwitterionic minimum of Gly•$(H_2O)_4$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol
47	1643.38	368.16471	47	1630.26	439.14693	47	1643.33	367.20209
48	1664.87	7.98409	48	1660.78	7.49027	48	1664.73	8.00852
49	1673.87	145.07989	49	1667.56	139.82815	49	1673.86	145.31893
50	1695.04	104.03017	50	1687.64	90.98999	50	1694.71	102.31982
51	1717.36	12.49064	51	1712.87	19.47912	51	1717.32	12.16055
52	1732.68	64.60973	52	1723.98	55.07693	52	1731.91	57.67309
53	1752.75	137.98192	53	1746.90	52.71622	53	1751.98	146.56515
54	2677.48	1197.98926	54	2677.38	1196.32539	54	2670.35	1202.24469
55	3115.69	362.47233	55	3114.91	354.53809	55	3109.67	384.50333
56	3133.19	38.97995	56	3133.09	34.08214	56	3132.71	22.14866
57	3210.84	0.38193	57	3210.84	0.44600	57	3210.84	0.40888
58	3350.80	1317.84973	58	3341.05	1334.98846	58	3350.38	1307.82472
59	3394.47	336.39311	59	3383.58	324.50007	59	3394.46	337.29802
60	3461.43	535.17714	60	3451.38	543.43447	60	3461.39	534.08421
61	3531.22	595.16201	61	3521.38	606.12066	61	3531.20	597.19852
62	3565.13	32.18501	62	3565.07	30.47895	62	3557.13	30.81121
63	3601.19	697.98650	63	3588.14	679.75991	63	3601.17	696.47905
64	3911.38	80.52656	64	3898.49	75.92546	64	3911.38	80.53030
65	3915.82	99.27416	65	3902.99	93.32903	65	3915.82	99.34385
66	3921.71	88.93510	66	3908.78	83.80788	66	3921.71	88.93150

Table 116: Harmonic frequencies for the structure 5N8a, the global non–dissociated minimum of Gly•$(H_2O)_5$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol
1	-0.00	0.00000	1	-0.00	0.00000	1	-0.00	0.00000
2	-0.00	0.00000	2	-0.00	0.00000	2	-0.00	0.00000
3	-0.00	0.00000	3	-0.00	0.00000	3	-0.00	0.00000
4	-0.00	0.00000	4	0.00	0.00000	4	-0.00	0.00000
5	0.00	0.00000	5	0.00	0.00000	5	0.00	0.00000
6	0.00	0.00000	6	0.00	0.00000	6	0.00	0.00000
7	41.35	1.90082	7	39.58	1.73333	7	41.24	1.89080
8	57.81	1.40370	8	55.39	1.15314	8	57.74	1.43489
9	63.12	2.26041	9	60.12	2.20354	9	63.01	2.18422
10	70.81	1.03396	10	67.51	1.02912	10	70.68	0.89293
11	76.20	8.35516	11	73.15	7.57993	11	75.92	8.41969
12	88.44	3.80611	12	84.12	3.55407	12	88.40	3.82707
13	98.37	4.58785	13	93.73	4.22765	13	98.29	4.58266
14	131.84	2.93351	14	129.33	2.39784	14	131.46	2.92824
15	156.53	0.55641	15	148.89	0.62436	15	156.48	0.53699

Continued on next page...

Table 116: Harmonic frequencies for the structure 5N8a, the global non–dissociated minimum of Gly•$(H_2O)_5$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol
16	181.47	18.88692	16	175.24	16.82305	16	179.99	18.70208
17	186.91	6.50060	17	177.78	6.36092	17	186.80	6.41766
18	202.47	8.84831	18	194.78	10.20871	18	201.62	7.92227
19	221.07	12.42580	19	210.91	11.87929	19	220.87	13.11729
20	235.11	10.39583	20	226.16	12.00424	20	234.17	10.08262
21	254.28	55.59413	21	244.30	12.01084	21	254.28	55.55672
22	259.51	31.01140	22	253.76	70.69574	22	259.50	30.84371
23	294.33	121.55313	23	291.57	116.16376	23	294.31	121.87234
24	315.37	6.62583	24	308.18	8.23354	24	314.86	6.42541
25	325.81	36.41164	25	311.12	28.58886	25	325.53	37.46023
26	363.85	67.18324	26	359.51	64.53000	26	361.68	63.38721
27	391.04	84.34382	27	387.32	86.19212	27	390.62	87.33680
28	427.20	103.32957	28	426.30	103.47016	28	427.15	103.06800
29	453.21	51.37803	29	451.31	50.65150	29	453.07	52.17128
30	480.45	6.98391	30	471.76	6.35584	30	479.69	5.40162
31	486.45	12.24886	31	480.37	11.32354	31	484.09	14.12814
32	513.64	24.48320	32	512.51	25.00023	32	513.56	24.06699
33	558.85	25.39327	33	556.93	26.74216	33	558.82	25.40247
34	588.28	0.40353	34	575.63	0.42085	34	587.65	0.32178
35	628.51	21.53399	35	627.54	20.76543	35	628.14	21.65478
36	686.85	24.91258	36	675.16	24.13003	36	685.92	25.01892
37	699.95	221.30293	37	697.27	219.11755	37	699.91	221.17586
38	745.20	67.90806	38	743.79	70.10433	38	744.95	67.58875
39	820.67	293.25162	39	817.93	286.99786	39	820.54	291.17523
40	834.32	108.33362	40	830.09	102.91721	40	833.61	108.17155
41	882.19	17.86386	41	860.19	18.97260	41	881.75	15.90731
42	905.67	112.14053	42	904.44	108.53677	42	904.05	127.28152
43	924.54	112.54083	43	923.02	115.92221	43	923.40	104.58240
44	1048.14	16.56911	44	1046.81	15.37960	44	1043.79	15.59185
45	1063.83	79.65318	45	1062.11	79.69049	45	1063.55	77.81612
46	1095.37	8.62871	46	1092.80	11.73763	46	1086.40	7.07661
47	1138.17	70.81211	47	1135.46	71.19678	47	1138.16	70.67738
48	1189.29	39.63327	48	1185.91	46.97083	48	1186.81	39.17957
49	1306.79	16.09289	49	1302.87	63.63994	49	1304.23	13.39025
50	1333.97	180.52445	50	1319.34	120.31151	50	1333.56	182.77381
51	1426.56	29.59157	51	1425.40	25.41173	51	1424.75	31.00788
52	1481.12	38.87467	52	1473.45	43.82409	52	1480.82	38.37708
53	1505.56	5.06309	53	1504.64	4.75456	53	1505.36	4.92982
54	1639.84	48.58184	54	1639.69	49.08867	54	1636.14	47.44752
55	1670.86	166.63313	55	1664.48	173.07071	55	1670.86	166.80340
56	1677.89	56.02683	56	1671.44	59.63222	56	1677.89	55.89271
57	1696.37	66.59980	57	1690.41	65.23074	57	1696.37	66.59725
58	1703.06	56.37620	58	1696.30	63.24543	58	1703.06	56.45049
59	1732.02	34.31356	59	1726.27	33.56176	59	1732.01	34.30095
60	1777.27	242.51779	60	1748.54	211.68823	60	1777.27	242.53542
61	3042.98	728.80862	61	3032.75	748.99941	61	3042.98	728.74815
62	3053.20	70.50893	62	3053.07	45.90335	62	3053.20	70.55242

Continued on next page...

Table 116: Harmonic frequencies for the structure 5N8a, the global non–dissociated minimum of Gly•$(H_2O)_5$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol
63	3162.41	39.28103	63	3153.88	1563.34484	63	3162.40	39.15700
64	3164.39	1536.12764	64	3162.46	1.49522	64	3164.39	1536.26794
65	3432.90	774.79536	65	3422.23	772.57537	65	3432.90	774.78610
66	3501.16	409.19016	66	3491.19	415.47847	66	3500.97	406.67028
67	3528.61	557.33412	67	3518.12	559.82538	67	3528.60	553.63813
68	3543.23	14.41529	68	3542.95	9.40772	68	3538.41	20.19466
69	3625.08	520.03826	69	3612.58	506.36474	69	3625.07	525.74258
70	3639.29	14.94873	70	3639.28	16.22189	70	3629.17	9.21883
71	3707.15	236.13272	71	3698.56	234.84730	71	3707.15	236.12329
72	3781.72	342.89679	72	3767.12	339.10508	72	3781.72	342.89509
73	3885.01	89.78352	73	3872.18	84.86298	73	3885.01	89.78294
74	3904.48	68.07496	74	3891.91	64.91935	74	3904.48	68.07610
75	3924.08	74.63567	75	3911.10	70.19415	75	3924.08	74.63502

Table 117: Harmonic frequencies for the structure 5Za, the global zwitterionic minimum of Gly•$(H_2O)_5$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol
1	0.00	0.00000	1	-0.00	0.00000	1	-0.00	0.00000
2	0.00	0.00000	2	0.00	0.00000	2	-0.00	0.00000
3	0.00	0.00000	3	0.00	0.00000	3	-0.00	0.00000
4	0.00	0.00000	4	0.00	0.00000	4	-0.00	0.00000
5	0.00	0.00000	5	0.00	0.00000	5	-0.00	0.00000
6	0.00	0.00000	6	0.00	0.00000	6	-0.00	0.00000
7	58.77	3.48826	7	56.01	3.18167	7	58.74	3.47765
8	64.01	2.98177	8	61.04	2.63027	8	63.96	3.00531
9	77.99	2.46035	9	74.62	2.33512	9	77.70	2.45583
10	83.74	2.92492	10	79.78	2.68961	10	83.69	2.88308
11	90.97	0.18523	11	86.99	0.23426	11	90.83	0.18145
12	112.85	1.42009	12	107.99	1.26565	12	112.56	1.39557
13	152.26	3.08259	13	145.18	2.63112	13	152.09	3.21261
14	156.25	4.60649	14	148.86	3.88220	14	156.17	4.56654
15	186.60	3.17016	15	178.91	3.99124	15	186.24	2.90365
16	192.05	5.69203	16	183.07	4.34286	16	191.72	5.99116
17	204.18	5.13877	17	194.59	5.09474	17	204.00	5.07319
18	227.56	18.09486	18	216.47	16.73302	18	227.55	18.06877
19	251.95	18.23681	19	241.45	15.83464	19	251.73	18.32940
20	277.86	56.69634	20	265.73	52.77444	20	277.07	54.37555
21	289.59	52.02393	21	281.66	48.93620	21	289.03	53.71894
22	302.37	90.73318	22	293.14	72.65075	22	299.74	88.74412

Continued on next page...

Table 117: Harmonic frequencies for the structure 5Za, the global zwitterionic minimum of Gly•$(H_2O)_5$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol
23	307.69	15.03386	23	299.71	26.00765	23	307.55	13.29738
24	340.10	20.42378	24	337.22	25.04373	24	339.95	22.84512
25	355.88	47.45596	25	348.85	47.06346	25	350.52	43.32096
26	442.97	6.47899	26	431.94	6.64040	26	442.43	6.65584
27	467.88	61.38052	27	466.21	59.79190	27	467.74	60.81635
28	478.41	7.17497	28	476.65	9.21893	28	478.30	7.42946
29	511.81	67.97817	29	510.67	68.44644	29	511.36	68.79468
30	552.48	39.40496	30	551.21	39.59912	30	552.32	39.67928
31	560.67	95.01531	31	558.96	92.92997	31	560.63	94.96029
32	588.19	27.56250	32	586.56	27.39425	32	588.16	27.51854
33	629.35	98.86006	33	616.00	72.76791	33	629.01	97.55145
34	644.68	41.73395	34	640.91	68.01089	34	644.57	42.82772
35	705.79	18.31573	35	704.08	18.11115	35	705.49	18.20400
36	727.23	62.09321	36	725.03	64.46896	36	727.20	62.30387
37	773.09	67.99977	37	766.40	33.01716	37	772.05	56.64499
38	782.13	265.69171	38	778.07	275.58334	38	781.58	270.48269
39	813.72	243.24511	39	809.33	272.98868	39	813.29	251.74188
40	830.67	146.95807	40	827.43	130.07193	40	830.43	144.76381
41	876.49	180.45194	41	867.11	127.69525	41	876.16	181.30644
42	903.72	18.34852	42	888.38	61.11091	42	903.44	19.16343
43	982.90	2.97308	43	979.75	3.01136	43	982.83	3.03048
44	1028.36	3.62050	44	1026.05	5.60217	44	1017.91	3.36654
45	1044.58	74.16282	45	1042.53	71.69660	45	1044.57	73.99774
46	1155.01	24.98853	46	1153.37	25.89591	46	1151.89	27.47769
47	1162.15	13.35898	47	1161.42	14.77632	47	1160.30	12.91982
48	1352.77	40.52095	48	1334.47	68.61131	48	1349.08	1.93144
49	1354.59	0.18745	49	1354.26	0.66938	49	1351.70	37.62661
50	1425.56	104.67038	50	1410.55	72.24367	50	1424.68	104.97362
51	1508.56	2.78426	51	1508.51	3.17464	51	1508.34	2.92146
52	1632.81	131.11378	52	1631.36	185.07745	52	1627.25	124.28090
53	1662.99	347.17140	53	1652.22	398.92836	53	1662.91	352.45037
54	1681.90	96.62158	54	1673.62	104.74413	54	1681.78	96.06433
55	1688.90	77.37031	55	1683.87	64.68541	55	1688.79	79.79272
56	1697.56	70.89352	56	1687.88	8.47909	56	1697.38	70.90137
57	1716.68	33.44687	57	1710.45	36.14508	57	1716.65	33.03902
58	1727.12	90.38578	58	1720.79	50.27902	58	1727.02	90.73979
59	1746.47	35.28628	59	1740.06	52.88238	59	1746.03	24.95692
60	1753.88	160.39086	60	1751.52	108.79797	60	1752.76	172.14204
61	2825.17	889.57707	61	2824.99	887.13913	61	2816.37	891.06737
62	2885.80	866.78353	62	2885.69	863.54098	62	2880.65	867.04726
63	3133.05	6.30196	63	3132.94	80.81975	63	3133.05	6.31790
64	3145.01	888.33106	64	3134.56	809.68215	64	3145.00	888.06662
65	3211.61	3.20835	65	3211.60	3.22525	65	3211.60	3.21115
66	3320.82	718.78846	66	3310.10	717.85861	66	3320.81	717.82522
67	3505.00	643.90896	67	3494.41	640.40426	67	3504.99	643.84979
68	3556.95	378.46974	68	3547.64	412.35180	68	3554.89	235.06918
69	3566.76	120.42571	69	3566.08	100.52844	69	3560.89	254.15414

Continued on next page...

Table 117: Harmonic frequencies for the structure 5Za, the global zwitterionic minimum of Gly•$(H_2O)_5$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol
70	3594.60	261.84935	70	3586.92	249.43258	70	3594.49	268.57637
71	3647.26	502.01296	71	3632.42	517.61277	71	3647.26	501.67311
72	3697.64	539.06662	72	3684.88	518.30605	72	3697.63	539.43696
73	3760.89	299.10166	73	3748.62	291.55728	73	3760.89	299.06448
74	3907.20	68.02193	74	3894.60	64.29630	74	3907.20	68.02247
75	3913.90	89.53000	75	3901.13	83.87703	75	3913.90	89.52961

Table 118: Harmonic frequencies for the structure 6N6a, the global non–dissociated minimum of Gly•$(H_2O)_6$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol
1	-0.00	0.00000	1	-0.00	0.00000	1	0.00	0.00000
2	0.00	0.00000	2	-0.00	0.00000	2	0.00	0.00000
3	0.00	0.00000	3	-0.00	0.00000	3	0.00	0.00000
4	0.00	0.00000	4	-0.00	0.00000	4	0.00	0.00000
5	0.00	0.00000	5	0.00	0.00000	5	0.00	0.00000
6	0.00	0.00000	6	0.00	0.00000	6	0.00	0.00000
7	54.75	2.81658	7	52.38	2.56009	7	54.61	2.79529
8	64.38	1.69899	8	61.05	1.45733	8	64.37	1.70994
9	65.19	0.36913	9	61.95	0.39353	9	65.18	0.35591
10	67.97	1.07265	10	65.16	1.02907	10	67.66	1.03871
11	74.56	0.86665	11	71.11	0.80247	11	74.43	0.88427
12	79.52	2.09735	12	75.65	1.93554	12	79.47	2.08206
13	97.06	1.64810	13	92.74	1.60915	13	96.78	1.57684
14	100.35	1.48426	14	95.45	1.20921	14	100.22	1.52818
15	140.61	3.55972	15	135.81	1.85089	15	140.52	3.54627
16	142.90	1.37975	16	137.91	2.95592	16	142.86	1.38889
17	159.46	1.68966	17	152.71	1.02561	17	158.97	1.80024
18	177.24	4.50011	18	169.13	3.00268	18	177.03	5.24200
19	183.80	6.57159	19	176.46	5.80727	19	182.91	6.29178
20	207.84	26.96333	20	199.53	26.40108	20	207.13	25.66008
21	215.65	5.01079	21	207.52	6.68136	21	214.82	4.74287
22	225.46	3.31571	22	215.22	5.35628	22	225.34	3.49193
23	252.72	74.92067	23	247.15	8.60964	23	252.71	74.72991
24	260.58	9.20596	24	250.29	68.35777	24	260.58	9.13251
25	274.31	38.02985	25	269.65	39.73016	25	273.66	39.03317
26	289.33	65.64019	26	283.51	58.82038	26	289.30	65.28232
27	310.55	19.49552	27	299.18	22.59830	27	310.48	19.38002
28	317.48	17.11568	28	302.77	13.19848	28	317.06	17.26947
29	327.56	67.27200	29	324.97	65.90699	29	327.34	65.42658

Continued on next page...

Table 118: Harmonic frequencies for the structure 6N6a, the global non–dissociated minimum of Gly•$(H_2O)_6$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol
30	353.88	16.12299	30	347.57	13.16974	30	351.18	17.89360
31	432.19	22.74631	31	431.17	23.81960	31	432.17	22.69800
32	447.75	69.50798	32	446.72	69.54727	32	447.73	69.31478
33	492.07	24.96151	33	484.85	4.60323	33	491.50	22.96190
34	498.85	2.33435	34	492.13	22.75295	34	496.15	4.42612
35	523.77	56.59978	35	521.30	57.69052	35	523.58	56.80148
36	546.08	51.76652	36	544.26	51.67040	36	545.98	51.75674
37	583.16	41.18325	37	578.13	17.01079	37	583.04	40.48167
38	597.72	66.92954	38	591.39	99.36208	38	597.46	66.78089
39	605.66	44.77052	39	604.21	39.53940	39	605.65	45.29577
40	643.68	8.73365	40	642.55	13.92449	40	643.39	8.93253
41	660.55	9.89368	41	644.84	2.63792	41	659.83	10.12474
42	714.15	315.51023	42	711.53	310.93334	42	714.02	314.99977
43	746.59	67.44108	43	745.51	69.07521	43	746.33	66.87399
44	793.55	204.16782	44	790.45	201.71902	44	793.47	203.96518
45	823.92	190.64649	45	820.66	181.67102	45	823.36	190.53561
46	880.68	22.35222	46	863.96	16.05634	46	880.36	21.81749
47	907.42	97.35487	47	904.77	99.70635	47	906.75	106.62807
48	918.62	133.17946	48	917.81	135.83542	48	915.90	128.85893
49	956.87	92.76159	49	951.75	90.47201	49	956.79	92.41347
50	1041.60	85.27722	50	1038.99	85.01787	50	1041.55	86.22627
51	1055.00	19.64445	51	1054.16	20.85180	51	1050.81	16.49823
52	1061.77	64.43132	52	1059.75	62.00322	52	1061.72	63.70681
53	1110.27	8.86570	53	1108.19	13.06118	53	1100.63	8.32306
54	1202.23	32.12687	54	1198.74	46.08225	54	1200.52	29.14601
55	1277.05	133.28532	55	1263.33	171.47594	55	1275.65	127.33107
56	1304.80	81.93296	56	1298.61	27.18453	56	1302.31	89.24300
57	1410.05	4.43901	57	1406.37	2.12218	57	1409.01	5.02533
58	1498.52	51.16023	58	1493.42	47.00992	58	1498.25	51.10669
59	1509.28	14.19833	59	1508.98	15.93069	59	1509.03	14.40260
60	1626.24	71.86011	60	1625.29	79.91758	60	1622.42	69.89953
61	1669.69	152.92805	61	1663.08	158.02738	61	1669.68	153.16034
62	1683.86	86.58807	62	1677.57	83.90066	62	1683.86	86.55778
63	1684.58	70.25162	63	1678.32	72.76725	63	1684.58	70.23887
64	1707.15	6.47006	64	1700.15	4.65167	64	1707.15	6.41787
65	1718.26	52.56390	65	1712.25	48.38909	65	1718.26	52.55454
66	1736.98	22.90796	66	1731.06	24.52686	66	1736.97	22.92613
67	1780.42	228.52069	67	1752.46	207.26686	67	1780.39	229.11035
68	3056.88	27.01898	68	3056.87	26.77391	68	3056.88	27.02596
69	3153.44	439.49327	69	3143.01	490.86116	69	3153.44	439.15323
70	3155.33	53.05318	70	3155.15	1.79640	70	3155.32	53.35363
71	3196.13	1259.60508	71	3185.62	1251.45328	71	3196.13	1259.63257
72	3326.40	934.19413	72	3315.41	926.76662	72	3326.40	934.19955
73	3451.06	963.39422	73	3440.44	961.65116	73	3451.06	963.36003
74	3510.53	420.84803	74	3501.10	435.45124	74	3510.03	408.32143
75	3539.82	32.38510	75	3539.22	20.05151	75	3535.25	44.48519
76	3616.11	502.69745	76	3603.28	494.97691	76	3616.10	503.50089

Continued on next page...

Table 118: Harmonic frequencies for the structure 6N6a, the global non–dissociated minimum of Gly•$(H_2O)_6$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol
77	3622.88	350.50993	77	3612.72	343.08362	77	3622.88	349.52103
78	3639.89	19.54547	78	3639.88	19.54002	78	3629.84	19.70587
79	3675.39	262.66386	79	3666.22	271.90130	79	3675.39	262.66046
80	3748.35	396.87657	80	3735.43	392.63909	80	3748.35	396.89957
81	3789.74	429.40676	81	3775.60	414.74760	81	3789.74	429.39891
82	3912.45	72.12841	82	3899.82	68.43950	82	3912.45	72.12958
83	3913.55	79.14092	83	3900.85	74.93098	83	3913.55	79.14126
84	3919.70	71.97316	84	3906.77	67.96534	84	3919.70	71.97246

Table 119: Harmonic frequencies for the structure 6Za, the global zwitterionic minimum of Gly•$(H_2O)_6$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol
1	0.00	0.00000	1	-0.00	0.00000	1	-0.00	0.00000
2	0.00	0.00000	2	-0.00	0.00000	2	-0.00	0.00000
3	0.00	0.00000	3	-0.00	0.00000	3	-0.00	0.00000
4	0.00	0.00000	4	-0.00	0.00000	4	-0.00	0.00000
5	0.00	0.00000	5	-0.00	0.00000	5	0.00	0.00000
6	0.00	0.00000	6	-0.00	0.00000	6	0.00	0.00000
7	52.67	1.00211	7	49.96	0.89404	7	52.66	1.00343
8	66.88	2.15115	8	63.87	1.65600	8	66.82	2.15732
9	69.98	2.68900	9	66.88	2.63591	9	69.90	2.72016
10	74.52	1.56674	10	71.07	1.28773	10	74.49	1.60475
11	79.92	4.68579	11	76.44	4.85828	11	79.68	4.56665
12	86.74	1.76624	12	82.67	1.29637	12	86.65	1.78691
13	105.31	0.55893	13	100.84	0.48885	13	105.01	0.54046
14	109.45	1.31167	14	104.26	1.20529	14	109.38	1.31425
15	139.70	8.23117	15	133.53	7.23472	15	139.47	8.23045
16	168.69	0.67773	16	161.09	0.50541	16	168.44	0.70897
17	175.31	2.52429	17	167.11	3.26883	17	175.21	2.37748
18	184.81	10.99326	18	177.02	8.81695	18	184.61	11.08023
19	204.09	3.43682	19	194.57	3.21654	19	204.02	3.50226
20	210.38	5.16172	20	199.91	5.15710	20	210.29	4.97473
21	233.21	17.94170	21	222.48	16.16857	21	233.19	17.78039
22	245.01	61.77421	22	234.46	60.56335	22	244.26	61.79815
23	256.47	39.63454	23	245.94	33.61906	23	255.75	40.22051
24	270.52	42.57665	24	267.88	36.67357	24	270.50	42.37897
25	313.63	64.89884	25	299.58	24.94856	25	312.00	94.20348
26	316.73	49.97031	26	308.63	88.64916	26	314.80	13.32355
27	342.14	18.58658	27	338.11	19.05615	27	341.81	21.66498

Continued on next page...

Table 119: Harmonic frequencies for the structure 6Za, the global zwitterionic minimum of Gly•$(H_2O)_6$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol
28	364.39	51.91301	28	355.28	54.23248	28	360.01	50.91637
29	386.19	42.90311	29	384.86	41.81651	29	386.15	41.59460
30	442.92	14.48526	30	438.69	11.80188	30	442.63	14.15833
31	447.38	72.16921	31	446.11	64.17520	31	447.25	73.27001
32	465.04	26.22576	32	455.43	39.83496	32	464.07	25.42183
33	498.11	36.17776	33	497.00	36.98945	33	498.04	36.39843
34	530.61	82.20286	34	528.84	80.85291	34	530.33	83.46611
35	540.41	60.94197	35	539.14	60.55882	35	540.06	60.69851
36	562.41	28.27563	36	558.87	24.15661	36	562.26	28.48094
37	626.15	59.21733	37	612.93	55.54995	37	625.57	59.76928
38	629.86	25.75792	38	628.72	29.85624	38	629.81	25.04000
39	656.86	60.33354	39	655.23	62.07380	39	656.85	60.39578
40	675.19	24.05936	40	673.41	24.01655	40	674.88	24.19725
41	721.32	295.38894	41	718.72	293.24578	41	721.32	295.60142
42	752.65	147.56874	42	748.92	49.26644	42	752.41	145.20581
43	760.48	31.36454	43	750.61	125.14323	43	758.96	32.85656
44	800.21	375.86479	44	797.40	377.13574	44	800.12	374.74328
45	839.10	88.35850	45	834.84	86.65610	45	838.82	89.96006
46	845.70	141.06365	46	843.24	136.43101	46	845.70	141.17657
47	902.99	76.27408	47	887.63	11.24086	47	902.60	74.34519
48	917.17	79.10623	48	909.19	132.40553	48	916.97	81.61918
49	988.28	8.46573	49	985.43	8.42040	49	988.06	8.40486
50	1019.61	70.95314	50	1017.46	68.39854	50	1019.58	70.94629
51	1045.56	4.21156	51	1043.02	6.22930	51	1035.30	4.10358
52	1160.20	16.22721	52	1158.97	16.74200	52	1155.97	18.80766
53	1167.02	10.42904	53	1165.94	11.87614	53	1166.24	9.75141
54	1351.27	7.17376	54	1341.27	71.24242	54	1346.19	6.43058
55	1358.79	42.24228	55	1351.13	6.00559	55	1357.69	41.62801
56	1437.80	109.94626	56	1422.04	78.42398	56	1437.02	110.01860
57	1506.67	3.97096	57	1506.60	4.71075	57	1506.50	4.18232
58	1632.15	194.20471	58	1629.90	289.48461	58	1626.38	181.03483
59	1660.31	226.22416	59	1649.56	248.68816	59	1660.17	237.04004
60	1673.98	181.30269	60	1665.55	166.94983	60	1673.85	179.72323
61	1684.37	102.50606	61	1677.67	99.56447	61	1684.25	104.69441
62	1694.81	85.26690	62	1686.43	15.05218	62	1694.59	87.72235
63	1706.00	70.93269	63	1700.08	63.24345	63	1705.96	70.94925
64	1713.85	23.24414	64	1709.62	13.37751	64	1713.81	22.78223
65	1721.87	80.86781	65	1713.93	61.47209	65	1721.84	80.93607
66	1751.96	43.85233	66	1745.48	38.15459	66	1751.69	39.05699
67	1763.95	130.57884	67	1762.50	106.98357	67	1762.59	137.13229
68	2649.07	1256.46144	68	2648.95	1254.75740	68	2641.55	1257.50160
69	2948.92	780.32805	69	2948.79	778.27155	69	2942.48	779.93495
70	3128.92	2.71474	70	3128.91	2.95134	70	3128.91	2.74532
71	3164.61	957.17343	71	3154.06	951.94005	71	3164.60	956.83607
72	3203.22	2.55421	72	3203.21	2.40529	72	3203.22	2.56510
73	3431.28	421.47853	73	3420.48	423.86978	73	3431.28	420.93763
74	3441.73	603.84710	74	3431.60	604.79402	74	3441.69	604.52611

Continued on next page...

Table 119: Harmonic frequencies for the structure 6Za, the global zwitterionic minimum of Gly•$(H_2O)_6$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol
75	3549.60	554.12724	75	3539.19	557.04371	75	3549.59	558.57796
76	3564.42	56.29341	76	3564.40	59.92887	76	3556.53	48.79724
77	3612.65	433.66894	77	3600.43	424.94539	77	3612.63	433.94422
78	3650.13	591.61798	78	3640.16	580.41023	78	3650.11	591.14324
79	3657.47	66.67180	79	3648.70	68.50225	79	3657.43	67.35989
80	3705.79	449.46729	80	3693.47	448.79677	80	3705.79	449.43236
81	3715.08	524.91664	81	3700.35	518.84690	81	3715.08	524.83345
82	3838.17	171.59842	82	3825.38	164.50992	82	3838.17	171.60017
83	3906.50	70.52622	83	3893.90	66.82689	83	3906.50	70.52684
84	3915.40	94.90489	84	3902.47	88.63737	84	3915.40	94.90598

Table 120: Harmonic frequencies for the structure 7N6a, the global non–dissociated minimum of Gly•$(H_2O)_7$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol
1	-0.00	0.00000	1	-0.00	0.00000	1	-0.00	0.00000
2	-0.00	0.00000	2	-0.00	0.00000	2	-0.00	0.00000
3	0.00	0.00000	3	0.00	0.00000	3	0.00	0.00000
4	0.00	0.00000	4	0.00	0.00000	4	0.00	0.00000
5	0.00	0.00000	5	0.00	0.00000	5	0.00	0.00000
6	0.00	0.00000	6	0.00	0.00000	6	0.00	0.00000
7	37.02	1.58004	7	35.44	1.46252	7	36.86	1.55660
8	46.35	0.42731	8	44.12	0.38901	8	46.32	0.42788
9	53.85	0.15866	9	51.43	0.17642	9	53.81	0.15940
10	63.61	0.81203	10	61.21	0.77787	10	63.47	0.79698
11	68.84	1.15883	11	65.61	1.01807	11	68.68	1.14581
12	78.68	0.75271	12	74.93	0.65073	12	78.57	0.76096
13	90.15	0.71043	13	86.28	0.62134	13	89.74	0.71479
14	96.05	2.65883	14	91.53	2.46503	14	95.84	2.61726
15	111.22	1.87794	15	107.48	1.20174	15	111.18	1.93819
16	117.42	1.10498	16	112.09	1.38559	16	117.25	1.10844
17	158.86	8.47233	17	152.06	5.95724	17	158.14	8.98993
18	161.29	3.79170	18	153.89	4.77632	18	161.08	3.34027
19	168.11	3.12019	19	160.14	2.38394	19	168.01	3.26594
20	171.07	0.24942	20	162.73	0.31509	20	171.06	0.24630
21	185.58	8.24638	21	177.35	6.61508	21	185.17	8.39991
22	196.45	13.13046	22	187.48	14.93074	22	196.06	12.03064
23	209.89	8.22126	23	199.67	9.00987	23	209.78	7.75190
24	213.45	10.10296	24	203.44	7.85440	24	213.23	10.76923
25	267.49	18.37242	25	259.08	19.38666	25	266.97	17.54252

Continued on next page...

Table 120: Harmonic frequencies for the structure 7N6a, the global non–dissociated minimum of Gly•$(H_2O)_7$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol
26	273.67	14.74478	26	268.60	17.47352	26	273.43	15.25220
27	283.86	8.27040	27	269.81	2.48619	27	283.84	8.46073
28	290.41	37.07507	28	280.98	43.53302	28	289.93	37.02843
29	302.20	63.90692	29	287.79	36.20249	29	301.97	65.84098
30	304.31	59.82927	30	294.58	53.90902	30	304.18	57.29542
31	317.03	37.49320	31	312.32	41.76457	31	316.96	36.39309
32	324.05	54.73092	32	320.63	64.15458	32	323.93	56.50724
33	357.68	4.89565	33	353.57	3.46469	33	354.86	4.91016
34	454.58	10.81090	34	453.53	10.26009	34	454.57	10.82620
35	468.53	53.65564	35	466.92	49.02251	35	468.48	52.73839
36	476.18	80.42374	36	474.83	70.41433	36	476.18	80.11095
37	492.20	16.63920	37	479.09	31.95274	37	489.70	17.96182
38	512.92	56.25632	38	511.88	56.01719	38	512.83	56.36372
39	553.73	16.51632	39	552.65	17.27175	39	553.70	16.41146
40	578.35	14.00420	40	571.89	7.83793	40	578.34	13.86307
41	592.14	3.14041	41	584.10	9.73016	41	591.63	3.49777
42	613.39	10.42934	42	611.51	10.95009	42	613.28	10.21506
43	628.33	24.78026	43	627.21	24.01845	43	628.05	25.16305
44	660.84	28.01385	44	657.51	27.70973	44	660.63	27.80167
45	677.03	35.71370	45	675.66	36.93293	45	677.02	35.72487
46	699.36	3.03918	46	688.81	4.08314	46	698.46	3.39440
47	725.21	196.23111	47	723.40	203.76704	47	725.17	195.69366
48	739.03	373.45246	48	736.52	364.25125	48	739.03	373.33917
49	757.78	204.48567	49	754.44	201.96255	49	757.73	203.47507
50	791.83	204.21822	50	789.65	194.46892	50	791.15	204.88907
51	831.38	149.56209	51	827.77	147.66919	51	831.29	149.99624
52	894.72	15.20261	52	874.84	10.35066	52	894.41	15.31369
53	919.25	78.59325	53	918.08	79.60822	53	916.22	82.30911
54	981.96	129.01124	54	980.09	127.04308	54	981.93	129.35573
55	985.48	89.28781	55	983.59	86.99654	55	985.47	88.85651
56	1055.03	26.24470	56	1053.91	24.78329	56	1050.45	25.72269
57	1074.16	87.72363	57	1072.37	87.19528	57	1074.14	87.34565
58	1101.25	16.26007	58	1099.37	19.44514	58	1091.78	7.27036
59	1117.30	129.34243	59	1114.62	131.01484	59	1117.04	134.60064
60	1188.98	21.47078	60	1186.38	27.96886	60	1187.37	19.97437
61	1289.78	62.33186	61	1281.26	153.38093	61	1287.46	53.81339
62	1319.19	171.36252	62	1305.79	81.44971	62	1317.31	178.64422
63	1418.64	28.46476	63	1415.12	18.39835	63	1417.49	30.31273
64	1506.90	10.82126	64	1503.19	28.68444	64	1506.65	11.33181
65	1510.63	37.34296	65	1508.18	18.16522	65	1510.53	36.82222
66	1625.33	86.94248	66	1624.38	97.54413	66	1621.51	84.98974
67	1671.19	112.94707	67	1665.00	121.52164	67	1671.19	112.94915
68	1672.86	90.76953	68	1666.56	78.58155	68	1672.86	90.80168
69	1683.51	45.42594	69	1676.89	48.55847	69	1683.51	45.57247
70	1703.86	8.36853	70	1698.07	12.55514	70	1703.86	8.38740
71	1706.13	52.63615	71	1699.97	48.03436	71	1706.13	52.62088
72	1719.49	47.66863	72	1713.30	55.96181	72	1719.49	47.69562

Continued on next page...

Table 120: Harmonic frequencies for the structure 7N6a, the global non–dissociated minimum of Gly•$(H_2O)_7$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number	IR intensity	mode	wave number	IR intensity	mode	wave number	IR intensity
	cm^{-1}	km/mol		cm^{-1}	km/mol		cm^{-1}	km/mol
73	1740.27	10.61567	73	1734.52	8.19499	73	1740.27	10.61133
74	1776.33	305.30210	74	1747.29	273.35257	74	1776.29	306.11343
75	2979.63	1299.21708	75	2969.23	1290.00538	75	2979.63	1299.21346
76	3055.55	31.88866	76	3055.54	31.43886	76	3055.55	31.90026
77	3166.98	4.74930	77	3166.98	4.68359	77	3166.97	4.75232
78	3217.81	244.08095	78	3207.25	242.62444	78	3217.81	244.07754
79	3273.56	1292.25643	79	3263.04	1284.95034	79	3273.56	1292.22540
80	3281.95	1327.15082	80	3271.34	1319.59583	80	3281.95	1327.13243
81	3514.93	386.01355	81	3505.86	430.09042	81	3513.92	351.88210
82	3536.15	58.01262	82	3535.00	27.35447	82	3532.09	92.09262
83	3631.16	316.72597	83	3622.78	316.29174	83	3623.77	15.56604
84	3633.78	15.38985	84	3633.77	13.27399	84	3631.16	316.80122
85	3651.79	357.59883	85	3642.63	396.28612	85	3651.79	357.34285
86	3668.56	279.41282	86	3656.06	215.98606	86	3668.55	279.02112
87	3670.67	136.11229	87	3661.07	135.75031	87	3670.67	136.14234
88	3699.71	274.94688	88	3686.64	273.94237	88	3699.71	274.96777
89	3721.88	680.23508	89	3706.90	674.55075	89	3721.88	680.16648
90	3749.18	1070.32701	90	3734.32	1067.08179	90	3749.18	1070.34793
91	3912.09	76.69349	91	3899.41	72.90117	91	3912.09	76.69440
92	3913.53	73.90890	92	3900.83	69.78571	92	3913.53	73.90880
93	3914.94	70.06223	93	3902.18	66.36416	93	3914.94	70.06239

Table 121: Harmonic frequencies for the structure 7Zb, the global zwitterionic minimum of Gly•$(H_2O)_7$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number	IR intensity	mode	wave number	IR intensity	mode	wave number	IR intensity
	cm^{-1}	km/mol		cm^{-1}	km/mol		cm^{-1}	km/mol
1	-0.00	0.00000	1	-0.00	0.00000	1	-0.00	0.00000
2	0.00	0.00000	2	0.00	0.00000	2	0.00	0.00000
3	0.00	0.00000	3	0.00	0.00000	3	0.00	0.00000
4	0.00	0.00000	4	0.00	0.00000	4	0.00	0.00000
5	0.00	0.00000	5	0.00	0.00000	5	0.00	0.00000
6	0.00	0.00000	6	0.00	0.00000	6	0.00	0.00000
7	51.74	0.12421	7	49.31	0.11093	7	51.73	0.12426
8	56.72	5.84422	8	54.01	5.23581	8	56.64	5.84446
9	63.62	0.71050	9	60.49	0.63691	9	63.60	0.70661
10	67.56	0.29897	10	64.48	0.28085	10	67.47	0.30439
11	72.74	1.06580	11	69.18	1.02324	11	72.73	1.08828
12	76.57	9.07802	12	73.41	8.32088	12	76.29	8.95468
13	87.91	0.37561	13	83.30	0.31987	13	87.89	0.38607
14	109.23	1.24117	14	104.57	0.76090	14	109.19	1.26832

Continued on next page...

Table 121: Harmonic frequencies for the structure 7Zb, the global zwitterionic minimum of Gly•$(H_2O)_7$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number	IR intensity	mode	wave number	IR intensity	mode	wave number	IR intensity
	cm^{-1}	km/mol		cm^{-1}	km/mol		cm^{-1}	km/mol
15	115.56	3.55862	15	110.55	3.82499	15	115.37	3.47998
16	158.12	4.64411	16	151.00	3.93317	16	157.91	4.77496
17	163.78	2.31268	17	155.94	2.22453	17	163.64	2.25134
18	169.81	0.21664	18	161.88	0.10483	18	169.71	0.25084
19	173.04	4.09301	19	164.73	3.53995	19	173.03	4.10772
20	187.38	6.26168	20	179.46	7.97665	20	186.96	5.72613
21	192.61	5.94552	21	184.19	4.00356	21	192.26	6.34424
22	206.69	21.42157	22	196.59	19.34905	22	206.56	21.53073
23	220.55	10.50648	23	209.80	9.13470	23	220.49	10.73176
24	238.79	39.28481	24	227.71	35.83550	24	238.57	38.91653
25	270.85	10.07958	25	262.61	15.73734	25	269.45	12.90456
26	280.06	52.86149	26	276.14	47.10860	26	279.68	50.02171
27	310.57	71.90923	27	299.73	51.25475	27	309.08	72.65471
28	322.34	34.78949	28	307.77	43.29906	28	321.83	31.05698
29	326.83	33.15782	29	320.88	11.57691	29	326.62	33.82747
30	338.40	23.58384	30	326.22	37.51817	30	337.62	22.04615
31	346.34	44.43032	31	342.96	58.31882	31	346.17	48.14526
32	365.15	43.36314	32	356.53	39.30579	32	361.02	38.04819
33	453.33	42.40921	33	451.58	40.10731	33	453.14	42.65057
34	466.16	17.72639	34	463.86	12.51378	34	465.89	16.42624
35	478.91	10.59528	35	468.97	14.44661	35	477.14	10.69202
36	497.68	42.65957	36	495.76	47.09362	36	497.06	44.61614
37	509.08	92.13752	37	507.63	90.28075	37	509.05	91.66274
38	531.56	31.61668	38	529.80	32.42186	38	531.53	31.39553
39	556.49	52.10676	39	555.01	50.70347	39	556.37	52.26588
40	595.92	11.80452	40	591.71	15.84660	40	595.82	11.38544
41	610.36	59.73677	41	601.39	57.94824	41	609.78	59.94290
42	629.28	10.80113	42	627.08	11.38697	42	629.22	10.84008
43	655.92	60.86108	43	654.55	59.98116	43	655.90	60.53055
44	671.08	36.93923	44	669.86	35.44673	44	671.05	36.62855
45	690.58	59.57405	45	683.91	53.58018	45	690.37	60.18555
46	731.85	21.33528	46	725.38	21.71454	46	731.06	20.78927
47	762.48	141.10280	47	759.43	148.89599	47	762.44	140.10498
48	778.33	63.17672	48	775.47	55.68441	48	778.08	62.15249
49	799.36	358.31883	49	795.17	352.41700	49	798.80	360.61202
50	823.84	326.12749	50	820.67	319.41297	50	823.80	325.33742
51	853.09	170.68716	51	846.53	156.80263	51	852.84	172.58482
52	896.76	9.29551	52	880.31	22.78894	52	896.42	9.34622
53	973.66	31.75835	53	968.05	26.76069	53	973.31	32.33626
54	979.38	9.75256	54	977.34	9.12088	54	979.28	9.74141
55	1049.34	6.14073	55	1046.28	8.16300	55	1040.05	3.72800
56	1054.64	95.90203	56	1052.61	95.75836	56	1054.56	97.75633
57	1084.78	100.49858	57	1082.57	99.21382	57	1084.75	99.86998
58	1155.33	25.46427	58	1153.71	27.04616	58	1150.88	27.66677
59	1165.78	4.38683	59	1165.17	4.77374	59	1164.33	4.50262
60	1350.56	4.22657	60	1338.26	85.09121	60	1345.56	2.82952
61	1355.63	48.07042	61	1350.59	2.51098	61	1354.58	47.91182

Continued on next page...

Table 121: Harmonic frequencies for the structure 7Zb, the global zwitterionic minimum of Gly•$(H_2O)_7$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number	IR intensity	mode	wave number	IR intensity	mode	wave number	IR intensity
	cm^{-1}	km/mol		cm^{-1}	km/mol		cm^{-1}	km/mol
62	1421.25	150.23846	62	1407.26	102.53073	62	1420.35	151.15433
63	1499.78	1.43153	63	1499.50	2.61687	63	1499.58	1.58631
64	1640.09	137.26991	64	1638.69	183.57806	64	1634.15	133.16529
65	1669.19	172.75183	65	1661.30	227.12949	65	1669.19	173.72711
66	1677.30	117.81672	66	1671.10	101.44488	66	1677.28	117.77339
67	1690.18	36.40277	67	1679.04	149.75714	67	1689.69	35.31813
68	1693.22	58.20090	68	1688.12	57.47253	68	1693.11	59.78452
69	1705.75	262.38307	69	1694.37	130.47264	69	1705.55	263.29928
70	1714.73	20.62074	70	1708.36	30.34939	70	1714.71	20.96459
71	1720.26	51.30807	71	1713.76	49.46029	71	1720.25	51.56315
72	1724.17	92.62481	72	1717.61	27.79527	72	1724.02	92.10926
73	1745.82	136.22568	73	1740.58	94.37334	73	1745.49	146.13762
74	1757.23	44.12170	74	1755.05	48.71496	74	1756.23	37.99370
75	2795.68	1046.90766	75	2795.53	1042.16264	75	2787.86	1047.68041
76	2940.93	775.33956	76	2940.75	771.81331	76	2934.87	777.87754
77	3088.01	1334.45363	77	3077.59	1332.39076	77	3087.97	1331.75855
78	3128.87	1.12092	78	3128.87	1.23282	78	3128.87	1.15735
79	3171.68	575.76167	79	3161.16	572.48164	79	3171.67	575.37845
80	3204.67	5.96112	80	3204.64	9.96092	80	3204.67	5.97022
81	3235.99	1399.00902	81	3225.31	1388.70859	81	3235.99	1398.79848
82	3500.95	691.92583	82	3490.36	693.79978	82	3500.95	691.58843
83	3550.87	602.57251	83	3541.74	595.03909	83	3549.83	561.47669
84	3562.58	4.99097	84	3562.18	21.73581	84	3555.74	43.66672
85	3608.52	299.73244	85	3599.64	292.42049	85	3608.40	300.41118
86	3625.54	226.57700	86	3616.70	219.56041	86	3625.54	226.27701
87	3637.38	343.63082	87	3624.08	361.68450	87	3637.37	343.17961
88	3691.64	689.76446	88	3677.72	652.58604	88	3691.63	689.79622
89	3696.51	509.00167	89	3682.61	523.77108	89	3696.51	509.09337
90	3751.98	389.78938	90	3739.71	376.11878	90	3751.98	389.74664
91	3905.40	65.48862	91	3892.83	62.39542	91	3905.40	65.48903
92	3906.23	71.45993	92	3893.70	67.75529	92	3906.23	71.46096
93	3915.71	80.32301	93	3903.00	75.49381	93	3915.71	80.32261

Table 122: Harmonic frequencies for the structure 8N8a, the global non–dissociated minimum of Gly•$(H_2O)_8$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number	IR intensity	mode	wave number	IR intensity	mode	wave number	IR intensity
	cm^{-1}	km/mol		cm^{-1}	km/mol		cm^{-1}	km/mol
1	-0.00	0.00000	1	-0.00	0.00000	1	-0.00	0.00000
2	0.00	0.00000	2	-0.00	0.00000	2	-0.00	0.00000
3	0.00	0.00000	3	-0.00	0.00000	3	-0.00	0.00000

Continued on next page...

Table 122: Harmonic frequencies for the structure 8N8a, the global non–dissociated minimum of Gly•$(H_2O)_8$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol
4	0.00	0.00000	4	-0.00	0.00000	4	-0.00	0.00000
5	0.00	0.00000	5	0.00	0.00000	5	-0.00	0.00000
6	0.00	0.00000	6	0.00	0.00000	6	0.00	0.00000
7	44.73	0.39537	7	43.06	0.40106	7	44.72	0.39182
8	52.68	1.81146	8	50.59	1.70059	8	52.46	1.77716
9	56.93	0.26220	9	54.17	0.20026	9	56.87	0.27135
10	66.38	0.76449	10	62.93	0.69203	10	66.37	0.76137
11	67.89	0.19913	11	64.59	0.18442	11	67.86	0.19723
12	70.90	0.53318	12	67.61	0.48487	12	70.73	0.52617
13	81.20	2.75419	13	77.09	2.45000	13	81.17	2.76677
14	91.92	1.36281	14	87.87	1.21822	14	91.57	1.34945
15	97.70	3.07983	15	92.78	2.91020	15	97.63	3.04447
16	113.05	1.50556	16	108.44	1.42332	16	112.45	1.47952
17	116.70	0.48415	17	112.94	0.24252	17	116.56	0.53878
18	141.25	0.51958	18	135.08	0.42031	18	141.14	0.52687
19	159.82	1.37091	19	152.84	0.91298	19	159.24	1.56059
20	165.75	0.98688	20	157.68	0.77091	20	165.66	0.99695
21	175.52	8.21301	21	167.05	6.99889	21	175.42	8.16692
22	179.04	1.34332	22	170.43	1.25030	22	178.88	1.47312
23	186.03	4.49751	23	177.59	4.52890	23	185.71	4.42739
24	199.52	15.58368	24	190.93	14.58304	24	198.85	15.12049
25	206.69	20.07834	25	196.56	19.52731	25	206.62	19.77836
26	217.73	5.31050	26	207.78	6.24435	26	217.40	5.01350
27	250.11	28.21887	27	239.21	27.31391	27	249.37	27.75997
28	266.76	12.35765	28	256.24	10.25088	28	265.93	12.74555
29	290.21	19.77071	29	279.51	6.59543	29	290.10	19.83792
30	297.62	7.23018	30	286.92	26.84707	30	297.60	7.06246
31	306.33	89.18009	31	294.52	49.30419	31	306.30	89.12398
32	310.09	41.86506	32	301.74	48.19448	32	310.04	41.76212
33	314.23	3.73927	33	307.37	19.76764	33	314.01	3.89717
34	337.92	94.85479	34	335.30	87.52251	34	337.85	94.33317
35	344.72	9.32934	35	337.97	13.27815	35	344.37	9.10515
36	381.50	79.58001	36	372.23	75.89272	36	379.08	80.36748
37	442.59	19.62405	37	441.72	19.15792	37	442.57	19.47402
38	467.98	80.97565	38	466.71	80.91916	38	467.96	80.54377
39	472.12	36.66686	39	470.83	24.14053	39	472.10	35.40058
40	488.03	49.39462	40	475.30	57.78951	40	486.05	54.20383
41	494.17	6.72239	41	491.81	3.02589	41	493.69	4.05015
42	548.67	33.17642	42	547.32	29.28197	42	548.67	33.14752
43	557.86	7.45394	43	556.51	11.09676	43	557.85	7.47044
44	570.95	74.75875	44	567.70	70.64680	44	570.93	74.80896
45	600.40	5.59434	45	589.90	5.52491	45	599.79	5.01337
46	614.09	32.18793	46	610.94	35.37351	46	613.83	33.23683
47	629.23	7.17956	47	627.97	7.52628	47	629.22	7.16998
48	653.47	9.92380	48	652.77	9.71177	48	653.18	10.08604
49	675.42	23.03630	49	673.74	22.52679	49	675.41	23.04245
50	705.13	26.42383	50	693.46	26.25091	50	704.36	26.42932

Continued on next page...

Table 122: Harmonic frequencies for the structure 8N8a, the global non–dissociated minimum of Gly•$(H_2O)_8$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol
51	711.81	23.86004	51	709.92	24.00580	51	711.77	23.75290
52	721.97	206.17394	52	719.74	207.47132	52	721.93	206.07524
53	753.73	563.66970	53	751.01	560.61319	53	753.72	563.06378
54	784.00	198.25906	54	781.17	197.20476	54	783.90	197.17563
55	805.70	125.12772	55	803.32	122.10948	55	804.89	125.48223
56	824.58	96.94356	56	821.12	93.75447	56	824.49	97.75387
57	893.84	7.35353	57	872.87	6.93328	57	893.44	6.12522
58	921.42	121.27995	58	920.69	121.96287	58	918.69	125.69242
59	954.84	90.76714	59	948.28	86.08797	59	954.77	90.72197
60	980.39	90.79291	60	978.54	84.12012	60	980.37	90.84032
61	1019.76	73.22885	61	1017.86	71.88839	61	1019.65	72.47651
62	1052.55	32.64589	62	1051.51	32.77717	62	1047.49	31.59447
63	1070.76	65.93891	63	1068.92	65.17018	63	1070.70	64.14433
64	1097.25	3.43080	64	1094.85	5.52500	64	1088.50	3.10795
65	1190.83	20.66306	65	1188.45	25.27942	65	1188.52	20.07454
66	1290.17	118.83664	66	1286.42	118.91170	66	1289.99	116.61408
67	1306.26	4.44334	67	1305.58	5.50886	67	1303.50	6.11714
68	1372.91	152.76669	68	1355.01	183.75276	68	1372.18	148.66454
69	1440.82	148.90608	69	1435.81	118.16115	69	1439.35	153.33200
70	1500.72	2.83341	70	1500.38	3.81806	70	1500.60	2.86409
71	1543.85	5.78991	71	1537.33	7.56701	71	1543.58	6.01651
72	1638.24	59.53401	72	1637.89	61.96614	72	1634.68	57.68056
73	1669.89	118.42843	73	1663.63	123.65628	73	1669.88	118.76848
74	1673.78	95.75975	74	1667.52	96.98139	74	1673.78	95.78280
75	1683.09	98.22703	75	1676.41	117.66005	75	1683.09	98.27478
76	1694.14	14.50775	76	1687.14	36.42454	76	1694.14	14.50057
77	1705.34	47.75446	77	1694.63	228.41216	77	1705.34	47.66306
78	1706.32	127.64072	78	1699.47	52.21384	78	1706.32	127.72162
79	1730.25	100.82419	79	1713.24	122.62570	79	1730.24	100.89827
80	1733.57	214.78614	80	1725.15	14.23253	80	1733.57	214.81455
81	1737.45	1.61002	81	1731.81	1.48608	81	1737.45	1.61398
82	2339.19	2181.17067	82	2329.03	2168.17611	82	2339.19	2181.18844
83	3053.77	25.41030	83	3053.76	25.47441	83	3053.77	25.41868
84	3160.65	4.94746	84	3160.65	4.92049	84	3160.64	4.95103
85	3223.96	478.61513	85	3213.47	472.88122	85	3223.96	478.65349
86	3247.06	890.86476	86	3236.46	889.36489	86	3247.06	890.82228
87	3288.38	1429.38730	87	3277.80	1419.10704	87	3288.38	1429.35097
88	3422.97	722.00330	88	3412.57	728.41318	88	3422.97	721.99163
89	3487.39	495.45888	89	3477.26	507.57875	89	3487.24	493.16098
90	3538.16	13.08366	90	3537.94	10.46147	90	3533.27	15.05588
91	3616.96	442.25473	91	3605.38	450.74293	91	3616.96	441.96004
92	3633.37	18.43605	92	3633.37	12.32807	92	3623.30	18.92007
93	3643.50	312.37962	93	3634.56	317.34604	93	3643.50	311.84896
94	3654.84	370.80980	94	3645.93	376.24645	94	3654.84	370.86455
95	3671.90	230.01021	95	3658.74	200.08000	95	3671.89	230.14500
96	3685.40	163.46025	96	3675.91	134.58300	96	3685.40	163.45836
97	3715.88	478.05634	97	3701.95	503.61425	97	3715.88	478.06358

Continued on next page...

Table 122: Harmonic frequencies for the structure 8N8a, the global non–dissociated minimum of Gly•$(H_2O)_8$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol
98	3729.82	704.27117	98	3715.25	699.61663	98	3729.82	704.26297
99	3777.41	785.00853	99	3763.01	764.37943	99	3777.41	785.02565
100	3905.87	79.11850	100	3893.24	75.25935	100	3905.87	79.11904
101	3913.17	91.25426	101	3900.45	85.84931	101	3913.17	91.25385
102	3913.38	55.43765	102	3900.64	53.14366	102	3913.38	55.43790

Table 123: Harmonic frequencies for the structure 8Za, the global zwitterionic minimum of Gly•$(H_2O)_8$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol
1	-0.00	0.00000	1	-0.00	0.00000	1	-0.00	0.00000
2	-0.00	0.00000	2	-0.00	0.00000	2	-0.00	0.00000
3	-0.00	0.00000	3	0.00	0.00000	3	-0.00	0.00000
4	0.00	0.00000	4	0.00	0.00000	4	0.00	0.00000
5	0.00	0.00000	5	0.00	0.00000	5	0.00	0.00000
6	0.00	0.00000	6	0.00	0.00000	6	0.00	0.00000
7	55.46	0.28216	7	52.64	0.24150	7	55.46	0.28264
8	57.36	0.46835	8	54.71	0.44907	8	57.33	0.46640
9	61.18	1.03250	9	58.30	0.80796	9	61.14	1.06304
10	62.37	0.17552	10	59.33	0.10903	10	62.31	0.18185
11	65.18	1.61602	11	62.13	1.54317	11	65.15	1.60673
12	71.75	2.59505	12	68.35	2.35701	12	71.63	2.61838
13	78.47	6.81236	13	74.85	6.23875	13	78.30	6.72993
14	92.69	0.50125	14	88.12	0.48115	14	92.62	0.50250
15	95.13	0.23096	15	90.37	0.26372	15	95.03	0.21706
16	106.21	1.63221	16	101.95	1.55339	16	105.98	1.61088
17	151.11	3.13809	17	144.72	2.94909	17	150.67	3.08518
18	161.39	1.29947	18	154.19	1.55569	18	161.37	1.32829
19	166.13	4.37109	19	158.42	3.40165	19	166.03	4.45380
20	174.38	9.69714	20	165.90	7.05319	20	174.29	9.86586
21	176.06	2.05596	21	167.75	3.25555	21	176.04	1.92981
22	184.35	2.40797	22	175.24	2.14323	22	184.33	2.37236
23	190.60	4.00908	23	182.22	3.91782	23	190.27	3.92272
24	208.79	9.87252	24	198.60	8.91628	24	208.76	10.01767
25	216.98	28.53879	25	206.39	24.52515	25	216.89	28.80054
26	225.16	17.46240	26	215.06	17.10080	26	224.82	17.05516
27	254.74	18.35277	27	246.18	18.74043	27	253.26	18.79330
28	271.84	35.22490	28	258.73	31.58805	28	271.46	35.35691
29	287.01	55.03110	29	280.66	52.24219	29	286.93	54.20423
30	304.59	15.64359	30	294.21	12.02550	30	304.56	15.67352

Continued on next page...

Table 123: Harmonic frequencies for the structure 8Za, the global zwitterionic minimum of Gly•$(H_2O)_8$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol
31	326.68	37.36554	31	315.77	14.63163	31	326.37	24.27824
32	329.99	49.80992	32	321.58	40.16110	32	327.37	77.73959
33	333.79	74.32001	33	324.80	98.50914	33	333.49	52.59879
34	346.04	25.13422	34	342.84	28.86813	34	345.91	28.30963
35	379.57	84.05528	35	369.04	82.99206	35	375.46	81.47390
36	449.91	32.54625	36	448.89	35.08313	36	449.77	33.25808
37	462.96	13.13064	37	457.25	2.29883	37	462.72	11.12390
38	467.92	26.43155	38	462.76	19.96084	38	467.02	24.69980
39	476.21	15.12140	39	472.68	29.81833	39	475.75	17.97791
40	512.46	67.14504	40	511.01	69.91111	40	511.98	68.60727
41	543.44	76.30486	41	541.75	73.68481	41	543.34	76.03448
42	547.37	32.93536	42	545.64	34.03385	42	547.30	32.78730
43	556.59	41.70592	43	554.54	41.01720	43	556.44	42.14409
44	598.67	11.09413	44	594.18	22.82798	44	598.46	11.27857
45	615.22	60.15269	45	604.59	44.73344	45	614.58	59.12244
46	629.20	23.02744	46	628.08	27.40214	46	629.15	22.87693
47	651.75	49.60439	47	650.68	50.46611	47	651.74	49.80688
48	663.72	74.79022	48	662.12	74.49286	48	663.61	74.97146
49	682.78	11.33627	49	680.93	13.74940	49	682.74	11.43626
50	686.85	24.29190	50	684.77	20.99248	50	686.64	24.55159
51	749.36	48.46502	51	740.09	38.42664	51	748.43	46.42281
52	757.55	189.82981	52	753.78	94.60151	52	757.52	180.52842
53	760.34	201.94066	53	755.98	297.00523	53	759.85	211.81603
54	767.58	324.63874	54	764.46	321.45606	54	767.49	325.24896
55	815.71	185.73711	55	812.95	185.80287	55	815.48	184.64722
56	835.64	159.37690	56	831.78	159.00408	56	835.53	161.38576
57	896.92	19.65412	57	879.37	8.84722	57	896.50	19.02424
58	933.36	68.05571	58	927.41	84.07810	58	933.13	69.04640
59	938.73	149.42408	59	935.83	130.36949	59	938.70	149.74642
60	994.58	21.84754	60	991.79	22.53982	60	994.30	21.89378
61	1042.29	32.02080	61	1040.42	31.53343	61	1042.24	31.84095
62	1056.10	43.53235	62	1053.68	33.74806	62	1046.91	6.85391
63	1059.61	104.73875	63	1057.21	113.25148	63	1058.80	141.21935
64	1159.61	16.22069	64	1158.08	17.16849	64	1155.73	18.77007
65	1170.05	9.30173	65	1169.20	10.28769	65	1168.59	8.85832
66	1340.97	10.64956	66	1340.67	11.27132	66	1336.06	10.27064
67	1361.99	50.55500	67	1344.87	81.72217	67	1361.00	49.40173
68	1438.21	134.25755	68	1422.95	94.78252	68	1437.43	134.51276
69	1503.60	3.06078	69	1503.42	4.41025	69	1503.41	3.29111
70	1637.44	186.68716	70	1635.20	277.37973	70	1631.64	177.23691
71	1671.53	248.84320	71	1659.99	382.54324	71	1671.51	255.22891
72	1676.21	167.07122	72	1667.02	71.62244	72	1675.96	164.52438
73	1680.41	92.36265	73	1674.29	90.69563	73	1680.40	92.70048
74	1685.91	75.58299	74	1679.19	74.31560	74	1685.78	78.27773
75	1695.26	111.63241	75	1685.49	7.63003	75	1694.99	115.47131
76	1708.91	65.44459	76	1703.43	44.72286	76	1708.85	65.18417
77	1716.07	54.29250	77	1710.44	42.09365	77	1716.00	53.03443

Continued on next page...

Table 123: Harmonic frequencies for the structure 8Za, the global zwitterionic minimum of Gly•$(H_2O)_8$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number	IR intensity	mode	wave number	IR intensity	mode	wave number	IR intensity
	cm^{-1}	km/mol		cm^{-1}	km/mol		cm^{-1}	km/mol
78	1719.39	3.19306	78	1714.54	2.28013	78	1719.37	3.35595
79	1729.58	25.02156	79	1723.68	24.52707	79	1729.57	25.05141
80	1746.61	63.62167	80	1740.59	49.66607	80	1746.60	63.89850
81	1761.49	95.48068	81	1760.71	88.83364	81	1760.00	97.30156
82	2536.90	1430.83436	82	2536.75	1429.50070	82	2529.54	1431.26219
83	3016.52	670.33862	83	3016.36	668.00964	83	3010.00	670.74812
84	3126.74	1.62504	84	3126.74	1.82802	84	3126.73	1.64478
85	3162.68	1049.14453	85	3152.20	1042.31236	85	3162.66	1048.84101
86	3186.41	750.75960	86	3175.83	746.22719	86	3186.41	750.57278
87	3201.03	2.72442	87	3201.02	2.88496	87	3201.03	2.74259
88	3286.09	1123.15023	88	3275.36	1118.78015	88	3286.09	1122.99827
89	3351.67	821.05471	89	3341.26	824.39522	89	3351.61	821.48650
90	3533.34	727.86311	90	3522.73	724.90560	90	3533.33	728.84006
91	3564.92	55.86715	91	3564.90	57.90066	91	3557.02	52.22363
92	3610.52	174.63783	92	3599.37	200.81677	92	3610.49	174.65985
93	3626.08	401.77472	93	3617.78	374.08725	93	3626.08	401.03692
94	3647.32	256.62877	94	3639.08	269.92575	94	3647.27	256.41221
95	3654.76	421.55972	95	3645.11	430.15967	95	3654.75	422.77009
96	3679.62	156.35961	96	3665.40	130.64689	96	3679.62	156.32759
97	3709.24	436.52303	97	3694.59	443.51767	97	3709.24	436.35980
98	3721.61	973.07175	98	3706.68	953.79716	98	3721.61	972.95103
99	3754.19	368.76218	99	3741.82	356.64804	99	3754.19	368.70610
100	3903.49	68.26089	100	3890.95	64.96962	100	3903.49	68.26157
101	3909.79	71.29379	101	3897.15	67.48749	101	3909.79	71.29417
102	3915.34	87.12004	102	3902.58	81.81468	102	3915.34	87.11983

Table 124: Harmonic frequencies for the structure gw9-6, the global non–dissociated minimum of Gly•$(H_2O)_9$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number	IR intensity	mode	wave number	IR intensity	mode	wave number	IR intensity
	cm^{-1}	km/mol		cm^{-1}	km/mol		cm^{-1}	km/mol
1	-0.00	0.00000	1	-0.00	0.00000	1	-0.00	0.00000
2	-0.00	0.00000	2	-0.00	0.00000	2	-0.00	0.00000
3	-0.00	0.00000	3	-0.00	0.00000	3	-0.00	0.00000
4	-0.00	0.00000	4	-0.00	0.00000	4	0.00	0.00000
5	-0.00	0.00000	5	0.00	0.00000	5	0.00	0.00000
6	-0.00	0.00000	6	0.00	0.00000	6	0.00	0.00000
7	28.93	3.36006	7	27.65	3.04713	7	28.88	3.35604
8	43.02	0.72081	8	41.20	0.70762	8	42.95	0.71585
9	51.14	0.30700	9	48.82	0.41390	9	51.04	0.28827
10	51.72	0.88907	10	49.36	0.80136	10	51.63	0.88783

Continued on next page...

Table 124: Harmonic frequencies for the structure gw9-6, the global non–dissociated minimum of Gly•$(H_2O)_9$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol
11	54.53	1.00982	11	52.29	0.80039	11	54.41	0.98903
12	58.65	1.37919	12	55.68	1.25527	12	58.62	1.36861
13	62.24	1.85800	13	59.17	1.63096	13	62.16	1.87517
14	69.20	0.76511	14	65.67	0.68975	14	69.20	0.76462
15	82.19	0.25702	15	78.11	0.22702	15	82.17	0.26296
16	88.78	2.75524	16	84.64	2.64284	16	88.53	2.66567
17	102.16	0.85875	17	97.63	0.86746	17	101.84	0.81735
18	107.78	2.64055	18	102.24	2.15688	18	107.69	2.73230
19	115.92	1.24864	19	112.84	1.11783	19	115.63	1.25226
20	148.57	0.28635	20	142.05	0.18558	20	148.14	0.34016
21	155.09	10.90462	21	147.90	9.49554	21	155.01	10.99953
22	163.12	0.16032	22	155.15	0.24365	22	163.09	0.15100
23	164.76	2.22268	23	156.60	2.05607	23	164.67	2.17037
24	169.49	0.42731	24	161.25	0.43502	24	169.45	0.41040
25	190.74	12.69757	25	182.00	9.92064	25	190.31	13.39630
26	198.85	37.68879	26	190.48	37.60394	26	198.16	35.61659
27	210.59	11.16265	27	200.09	10.08536	27	210.53	11.50768
28	212.87	1.62639	28	203.50	3.06321	28	212.40	1.11570
29	234.07	20.69854	29	225.26	19.46998	29	232.86	21.18979
30	254.00	25.33358	30	241.49	24.18731	30	253.97	25.14562
31	270.99	51.73810	31	266.94	26.76120	31	270.97	51.59625
32	279.24	20.10515	32	268.57	38.93310	32	278.64	20.94472
33	283.94	17.79890	33	281.02	19.33084	33	283.83	17.62536
34	315.19	40.25914	34	304.82	25.61609	34	315.09	40.18399
35	320.04	32.33936	35	308.32	25.37508	35	319.88	32.20002
36	325.01	23.72797	36	316.20	31.22715	36	324.98	23.71362
37	334.47	28.04492	37	319.71	13.02991	37	334.34	27.22745
38	337.38	44.23985	38	330.30	20.26496	38	337.36	44.22749
39	339.78	18.78617	39	335.47	59.69539	39	339.51	19.62752
40	376.54	39.52570	40	366.45	38.87851	40	374.27	39.80301
41	445.28	33.81705	41	444.02	32.99494	41	445.28	33.86646
42	466.41	55.69406	42	464.91	63.52067	42	466.39	56.07889
43	478.68	0.46272	43	467.27	14.04169	43	476.96	9.91708
44	481.37	62.60850	44	478.87	32.08347	44	480.65	51.69994
45	502.76	39.34457	45	501.57	43.08015	45	502.64	40.78173
46	518.16	23.26404	46	517.09	22.90288	46	518.15	23.30548
47	547.48	64.12450	47	545.74	62.87985	47	547.47	64.15877
48	586.04	28.29587	48	576.05	17.13201	48	585.76	27.09358
49	597.18	8.38023	49	593.13	24.38345	49	596.97	9.31630
50	610.03	59.77290	50	607.62	56.07390	50	609.93	60.00218
51	636.71	6.87531	51	634.73	7.81205	51	636.68	6.90660
52	656.23	8.11843	52	653.87	7.34231	52	655.93	7.82363
53	669.86	54.22546	53	669.09	55.24354	53	669.65	54.13008
54	690.31	43.68927	54	685.82	24.30594	54	690.19	43.45653
55	695.50	9.01888	55	691.33	23.94460	55	695.11	9.36228
56	706.74	20.59944	56	702.61	20.20655	56	706.56	20.60372
57	730.16	214.31084	57	726.98	232.12772	57	730.13	215.03795

Continued on next page...

Table 124: Harmonic frequencies for the structure gw9-6, the global non–dissociated minimum of Gly•$(H_2O)_9$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol
58	739.65	123.98066	58	737.08	118.62561	58	739.62	123.49540
59	758.01	338.40750	59	755.07	332.38498	59	758.01	338.69731
60	808.51	128.29678	60	806.63	117.97734	60	808.35	116.97566
61	812.81	136.12243	61	810.12	142.62841	61	811.79	147.75311
62	832.07	181.80998	62	828.74	175.41803	62	832.07	181.89616
63	889.24	101.71559	63	871.56	25.66273	63	889.04	99.38589
64	909.47	46.97283	64	900.59	113.58486	64	909.25	49.71737
65	920.58	101.85423	65	919.89	101.34390	65	917.77	102.25909
66	1014.29	70.41762	66	1012.31	69.46507	66	1014.07	70.35191
67	1033.12	30.07159	67	1031.12	29.24395	67	1033.10	29.89415
68	1055.19	23.18734	68	1053.96	22.38525	68	1049.72	21.26040
69	1089.16	138.70829	69	1087.14	136.94713	69	1087.22	3.02923
70	1095.67	6.70700	70	1093.20	8.56991	70	1089.30	142.28583
71	1159.03	138.71580	71	1155.61	139.10340	71	1158.96	137.78573
72	1189.77	24.70331	72	1187.17	30.09386	72	1187.47	23.75610
73	1305.30	3.58013	73	1304.80	7.11871	73	1302.36	3.20065
74	1355.56	202.08626	74	1336.61	212.97696	74	1355.10	199.13093
75	1431.99	105.22870	75	1429.10	84.63973	75	1430.22	108.68129
76	1503.98	1.76164	76	1503.68	2.24832	76	1503.86	1.77464
77	1541.31	15.43230	77	1535.45	16.79262	77	1541.01	15.86020
78	1638.74	49.72452	78	1638.47	50.94582	78	1635.19	48.30587
79	1673.49	109.52181	79	1667.02	108.53338	79	1673.49	109.26340
80	1676.48	14.72096	80	1670.10	14.01895	80	1676.48	14.71925
81	1685.43	123.40621	81	1679.37	123.01780	81	1685.43	123.55578
82	1688.63	36.05436	82	1682.42	34.31108	82	1688.62	35.99642
83	1702.84	66.54034	83	1696.92	70.41752	83	1702.84	66.56760
84	1709.13	27.39259	84	1703.30	22.54997	84	1709.13	27.38185
85	1711.25	29.57720	85	1705.39	35.33730	85	1711.25	29.64089
86	1739.65	67.99360	86	1730.33	220.09734	86	1739.65	67.98505
87	1747.93	16.47308	87	1737.44	144.92510	87	1747.93	16.50933
88	1764.36	324.21611	88	1743.41	21.70654	88	1764.36	324.24798
89	2642.50	2219.96589	89	2632.07	2205.96001	89	2642.50	2219.95964
90	3054.38	33.32819	90	3054.38	33.66976	90	3054.38	33.33920
91	3128.84	824.06222	91	3118.37	820.96379	91	3128.84	824.06367
92	3168.13	4.59138	92	3168.13	4.48891	92	3168.12	4.59401
93	3200.74	1553.14335	93	3190.24	1546.26118	93	3200.74	1553.13091
94	3216.79	1237.78550	94	3206.27	1229.04346	94	3216.78	1237.80859
95	3417.54	444.43429	95	3406.77	437.75525	95	3417.54	444.41795
96	3460.95	507.24750	96	3450.58	513.93801	96	3460.89	507.09135
97	3477.12	1180.17132	97	3466.73	1188.64371	97	3477.12	1179.44341
98	3536.42	8.47912	98	3536.32	7.29501	98	3531.46	9.18863
99	3608.96	335.73731	99	3600.77	338.70495	99	3608.96	335.58459
100	3632.22	15.38728	100	3632.20	6.90216	100	3622.16	16.31407
101	3648.70	341.08006	101	3635.38	383.64683	101	3648.70	340.20928
102	3660.22	320.13381	102	3651.92	266.43065	102	3660.21	319.81541
103	3675.91	218.59609	103	3665.87	234.50253	103	3675.91	218.64670
104	3700.81	630.16602	104	3687.52	597.84327	104	3700.80	630.30491

Continued on next page...

Table 124: Harmonic frequencies for the structure gw9-6, the global non–dissociated minimum of Gly•$(H_2O)_9$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number	IR intensity	mode	wave number	IR intensity	mode	wave number	IR intensity
	cm^{-1}	km/mol		cm^{-1}	km/mol		cm^{-1}	km/mol
105	3712.83	450.96472	105	3698.44	486.27079	105	3712.83	450.95393
106	3745.09	461.98924	106	3732.15	425.98500	106	3745.09	461.99883
107	3773.71	667.37154	107	3759.45	658.24236	107	3773.71	667.37716
108	3908.96	73.90373	108	3896.36	70.29138	108	3908.96	73.90334
109	3910.16	61.50764	109	3897.56	58.54478	109	3910.16	61.50780
110	3912.58	76.56708	110	3899.93	72.70424	110	3912.58	76.56772
111	3915.93	92.20951	111	3902.90	87.33198	111	3915.93	92.20945

Table 125: Harmonic frequencies for the structure gw9-27, the global zwitterionic minimum of Gly•$(H_2O)_9$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number	IR intensity	mode	wave number	IR intensity	mode	wave number	IR intensity
	cm^{-1}	km/mol		cm^{-1}	km/mol		cm^{-1}	km/mol
1	-0.00	0.00000	1	-0.00	0.00000	1	-0.00	0.00000
2	-0.00	0.00000	2	-0.00	0.00000	2	-0.00	0.00000
3	-0.00	0.00000	3	-0.00	0.00000	3	-0.00	0.00000
4	0.00	0.00000	4	-0.00	0.00000	4	0.00	0.00000
5	0.00	0.00000	5	0.00	0.00000	5	0.00	0.00000
6	0.00	0.00000	6	0.00	0.00000	6	0.00	0.00000
7	27.45	2.81097	7	26.21	2.56904	7	27.42	2.80278
8	44.03	1.43397	8	42.04	1.30706	8	43.95	1.42897
9	50.31	2.21155	9	47.89	1.98052	9	50.28	2.20585
10	52.49	5.43097	10	49.95	4.82172	10	52.46	5.43738
11	59.94	1.28547	11	56.99	1.21490	11	59.89	1.26347
12	72.79	0.53283	12	69.10	0.49297	12	72.76	0.53028
13	75.39	0.33226	13	71.94	0.31353	13	75.16	0.33015
14	81.54	0.59624	14	77.43	0.52685	14	81.47	0.59907
15	86.30	2.51296	15	82.50	2.31705	15	86.02	2.52214
16	101.95	8.17212	16	97.29	3.95055	16	101.62	8.84632
17	103.75	2.62900	17	98.86	5.65620	17	103.67	1.94457
18	131.82	7.36846	18	125.11	6.55117	18	131.78	7.33012
19	150.21	4.11566	19	146.09	5.81577	19	149.94	4.18620
20	155.57	1.04970	20	148.09	0.10363	20	155.57	1.03796
21	164.84	4.43875	21	157.18	3.15875	21	164.83	4.44100
22	174.24	12.71320	22	165.56	10.16215	22	174.16	12.78788
23	184.45	1.36750	23	177.02	0.83740	23	184.40	1.42522
24	195.49	24.93464	24	186.97	3.94751	24	195.43	23.77563
25	197.33	12.20934	25	191.08	13.11842	25	197.02	8.17712
26	199.68	45.02844	26	192.01	51.66013	26	199.05	49.08993
27	208.91	8.83798	27	200.68	2.73589	27	208.85	9.30715
28	217.30	7.34619	28	209.74	18.00782	28	217.27	7.57317

Continued on next page...

Table 125: Harmonic frequencies for the structure gw9-27, the global zwitterionic minimum of Gly•$(H_2O)_9$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O\rightarrow^{18}O$ and $^{14}N\rightarrow^{15}N$ are included.

Bare spectrum			$^{16}O\rightarrow^{18}O$			$^{14}N\rightarrow^{15}N$		
mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol
29	220.89	18.59222	29	211.85	10.19484	29	220.58	16.63147
30	230.10	109.26035	30	224.44	101.18937	30	229.76	110.76593
31	238.91	21.28210	31	228.42	32.33527	31	238.49	20.71208
32	248.70	77.07929	32	238.11	77.99198	32	248.57	78.26815
33	270.00	40.73642	33	266.94	42.74198	33	270.00	40.67660
34	291.01	16.38711	34	276.42	17.11183	34	290.92	16.64694
35	313.06	56.65315	35	300.19	45.11162	35	311.75	54.90379
36	324.83	38.72993	36	311.70	6.78218	36	324.82	38.82839
37	326.25	4.91366	37	315.55	18.86495	37	325.41	3.51248
38	344.14	28.93671	38	334.45	48.58663	38	344.04	30.35405
39	363.85	97.37820	39	356.73	92.67583	39	359.91	92.80858
40	434.19	92.83535	40	432.79	89.68207	40	434.15	92.22504
41	457.47	58.91350	41	456.60	76.36583	41	457.13	66.39850
42	462.30	53.40707	42	460.19	47.38948	42	462.01	48.30549
43	490.07	41.27502	43	485.92	61.35358	43	489.79	43.92754
44	505.42	23.13869	44	495.21	5.86482	44	502.87	19.99874
45	518.77	13.13233	45	517.34	14.37994	45	518.69	12.75294
46	534.58	22.27504	46	533.11	23.19601	46	534.51	22.32324
47	539.30	33.55890	47	537.64	31.56516	47	539.27	33.54335
48	549.25	43.47569	48	547.70	44.85324	48	549.23	43.11765
49	590.71	99.83070	49	589.27	97.26171	49	590.64	99.44352
50	610.95	59.55410	50	601.12	50.72952	50	610.50	57.70636
51	628.59	18.51730	51	625.48	26.56711	51	628.46	19.14786
52	634.63	45.94705	52	632.86	41.56993	52	634.57	44.99263
53	647.65	37.55014	53	646.43	39.18079	53	647.65	37.58074
54	691.29	28.32756	54	689.85	30.23306	54	691.26	28.80269
55	708.11	88.06594	55	698.40	36.47890	55	707.75	85.60167
56	719.03	41.97718	56	713.46	93.95206	56	718.61	44.92850
57	748.53	161.53541	57	746.65	158.90102	57	748.50	161.41913
58	767.03	213.15285	58	764.52	212.43184	58	766.98	213.62504
59	793.80	125.48979	59	791.40	122.41111	59	793.74	124.99633
60	806.84	123.38911	60	805.16	121.98332	60	806.83	123.37191
61	827.05	231.53173	61	823.14	222.29653	61	827.01	231.67719
62	881.37	45.69879	62	870.39	44.90116	62	881.21	46.00861
63	920.99	75.03865	63	908.23	29.25716	63	920.80	74.29042
64	922.33	74.60824	64	919.43	78.03527	64	922.00	74.15662
65	929.48	192.34814	65	926.21	220.43833	65	929.45	194.76864
66	950.67	163.16182	66	947.19	168.88346	66	950.60	162.68734
67	972.51	31.02992	67	970.18	29.25768	67	972.47	30.82880
68	1045.40	8.91902	68	1043.91	10.70613	68	1033.82	10.15553
69	1064.40	73.58020	69	1062.44	71.65964	69	1064.38	73.97022
70	1137.72	15.90759	70	1136.43	16.74970	70	1136.75	16.66878
71	1180.24	25.80202	71	1179.66	25.71788	71	1176.32	27.98327
72	1358.33	19.53839	72	1345.11	115.73815	72	1352.48	22.00055
73	1361.45	87.61760	73	1358.42	26.22752	73	1359.44	83.90280
74	1432.18	116.52040	74	1415.77	78.45152	74	1431.47	117.18803
75	1502.52	11.47897	75	1502.26	14.02301	75	1502.20	12.66089

Continued on next page...

Table 125: Harmonic frequencies for the structure gw9-27, the global zwitterionic minimum of Gly•$(H_2O)_9$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol
76	1542.13	172.57342	76	1541.32	179.87756	76	1536.33	170.70609
77	1646.47	102.34796	77	1640.15	174.66576	77	1646.02	102.93921
78	1667.49	131.14591	78	1660.75	228.25873	78	1667.49	133.28493
79	1669.37	163.89952	79	1662.41	78.90245	79	1669.33	162.09688
80	1673.35	84.57119	80	1667.71	73.64524	80	1673.31	85.73756
81	1686.31	40.65045	81	1679.92	24.96503	81	1686.30	40.43988
82	1704.49	204.90360	82	1688.16	154.10993	82	1704.39	205.40779
83	1705.97	34.28711	83	1699.42	37.11960	83	1705.96	33.15580
84	1715.04	161.90552	84	1708.43	137.92265	84	1715.02	161.50644
85	1732.13	65.22770	85	1725.96	57.22253	85	1732.11	61.06782
86	1735.73	61.03264	86	1732.40	61.16703	86	1734.69	64.77246
87	1742.88	40.20397	87	1737.94	15.84349	87	1742.69	42.97917
88	1758.20	15.88757	88	1754.00	18.22710	88	1757.88	15.16279
89	3060.04	367.94314	89	3059.56	347.85792	89	3053.92	387.35653
90	3139.09	29.68062	90	3136.63	853.79862	90	3139.00	27.92306
91	3147.84	1065.69056	91	3140.05	256.61183	91	3147.62	1045.95698
92	3190.35	704.60786	92	3189.77	696.52701	92	3183.48	717.90896
93	3211.73	7.80557	93	3211.72	7.16185	93	3211.66	4.40385
94	3313.86	432.57996	94	3302.97	425.04397	94	3313.84	433.44019
95	3356.19	1325.78099	95	3346.43	1317.18562	95	3356.17	1325.75201
96	3386.63	766.87824	96	3376.62	765.88762	96	3386.29	761.28315
97	3440.51	514.95584	97	3429.56	537.47631	97	3440.39	515.21674
98	3477.70	133.83786	98	3477.43	109.25927	98	3469.78	131.53564
99	3497.94	691.76049	99	3486.02	732.74414	99	3497.93	685.23436
100	3537.81	453.75215	100	3527.27	453.37944	100	3537.76	454.46734
101	3563.55	1112.92834	101	3553.54	1137.44564	101	3563.54	1115.27215
102	3574.95	609.28786	102	3562.95	541.33713	102	3574.94	608.73357
103	3605.01	222.51094	103	3594.79	236.59022	103	3605.01	222.59445
104	3672.00	294.94437	104	3663.42	292.37090	104	3672.00	294.84216
105	3727.06	101.32592	105	3714.51	83.97444	105	3727.06	101.34642
106	3753.76	642.56676	106	3739.24	645.47488	106	3753.76	642.57712
107	3785.88	245.64639	107	3772.97	236.20200	107	3785.87	245.52583
108	3909.96	68.57412	108	3897.35	65.02299	108	3909.96	68.57415
109	3914.97	92.06998	109	3902.19	86.24776	109	3914.97	92.08779
110	3927.89	89.40646	110	3914.93	84.39527	110	3927.89	89.47292
111	3929.20	101.00605	111	3915.91	94.96671	111	3929.20	101.00377

Table 126: Harmonic frequencies for the structure gw10-42, the global non–dissociated minimum of Gly•$(H_2O)_{10}$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number	IR intensity	mode	wave number	IR intensity	mode	wave number	IR intensity
	cm^{-1}	km/mol		cm^{-1}	km/mol		cm^{-1}	km/mol
1	-0.00	0.00000	1	-0.00	0.00000	1	-0.00	0.00000
2	-0.00	0.00000	2	-0.00	0.00000	2	-0.00	0.00000
3	0.00	0.00000	3	-0.00	0.00000	3	0.00	0.00000
4	0.00	0.00000	4	0.00	0.00000	4	0.00	0.00000
5	0.00	0.00000	5	0.00	0.00000	5	0.00	0.00000
6	0.00	0.00000	6	0.00	0.00000	6	0.00	0.00000
7	40.63	0.94095	7	38.84	0.91829	7	40.52	0.93077
8	45.30	1.66492	8	43.21	1.49166	8	45.26	1.66166
9	47.48	0.16281	9	45.16	0.08983	9	47.44	0.17391
10	52.99	1.68950	10	50.39	1.56687	10	52.97	1.68293
11	54.20	2.41459	11	52.02	2.30096	11	54.06	2.33229
12	60.48	1.26050	12	57.67	0.89854	12	60.31	1.38563
13	63.87	0.24436	13	60.89	0.17433	13	63.73	0.25082
14	66.41	1.47423	14	63.21	1.48182	14	66.32	1.40803
15	78.98	1.43471	15	74.84	1.27409	15	78.98	1.44038
16	82.28	1.49593	16	78.59	1.40484	16	82.09	1.44538
17	92.60	0.51096	17	88.37	0.43779	17	92.35	0.53962
18	95.86	0.77079	18	91.39	0.66974	18	95.70	0.77890
19	104.84	1.76143	19	99.37	1.55887	19	104.83	1.76235
20	121.34	0.80223	20	118.24	0.79367	20	121.12	0.79333
21	139.24	1.29105	21	132.41	1.02030	21	139.21	1.31187
22	145.39	0.61057	22	138.35	0.52579	22	145.36	0.61361
23	160.03	0.94295	23	152.19	0.87341	23	160.00	0.96781
24	172.86	1.14353	24	164.34	1.12862	24	172.81	1.03744
25	176.34	4.87167	25	167.58	3.39897	25	176.22	7.49304
26	176.95	7.60277	26	168.77	6.91133	26	176.62	5.58290
27	183.31	1.02867	27	174.93	1.10413	27	182.95	0.94529
28	191.55	27.36724	28	182.79	25.29817	28	191.36	27.04624
29	205.52	22.18556	29	196.57	29.79532	29	204.65	17.96523
30	208.83	15.19495	30	199.64	8.35130	30	208.57	18.24956
31	229.64	22.56010	31	218.57	18.41876	31	229.38	23.30161
32	237.52	28.36834	32	225.97	27.57314	32	237.48	28.17028
33	260.55	2.43936	33	249.33	2.80996	33	260.22	2.43646
34	271.27	49.81170	34	263.10	5.51486	34	271.00	31.56299
35	272.48	22.80026	35	268.54	61.54083	35	271.89	41.40617
36	308.09	93.62590	36	298.60	92.35720	36	307.72	98.15031
37	311.74	26.03044	37	301.32	13.93666	37	311.36	19.34315
38	320.80	3.97121	38	308.64	4.64791	38	320.79	3.91878
39	327.76	29.71081	39	316.21	20.78356	39	327.71	30.15584
40	330.68	28.15693	40	326.57	32.38308	40	330.67	28.13088
41	331.66	83.87392	41	329.20	91.54657	41	331.64	83.27521
42	362.08	23.96065	42	356.45	26.15704	42	359.36	24.62284
43	381.33	16.72126	43	365.08	10.57935	43	381.12	17.11327
44	436.34	37.82941	44	435.14	38.20656	44	436.32	37.92492
45	440.20	49.61679	45	439.07	50.21760	45	440.20	49.60524
46	469.57	38.98528	46	468.07	37.64473	46	469.55	38.82301

Continued on next page...

Table 126: Harmonic frequencies for the structure gw10-42, the global non–dissociated minimum of Gly•$(H_2O)_{10}$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol
47	487.59	59.59937	47	486.16	58.90970	47	487.57	59.57470
48	509.95	20.37414	48	495.99	20.99098	48	507.38	23.31999
49	517.37	33.22815	49	515.71	27.44443	49	517.31	31.53876
50	537.34	9.14230	50	535.89	9.40810	50	537.32	9.02257
51	550.09	57.61135	51	548.13	56.12572	51	549.84	57.79958
52	573.17	13.87253	52	571.63	14.13105	52	573.17	13.85306
53	585.33	33.09946	53	577.48	10.27356	53	585.19	31.63397
54	591.25	44.48819	54	588.40	65.75836	54	591.13	45.97288
55	608.57	17.69592	55	605.70	19.07418	55	608.28	17.08937
56	615.49	13.84471	56	613.78	16.58694	56	615.46	14.26801
57	654.42	56.58645	57	651.94	60.06367	57	654.33	57.26037
58	672.87	42.81877	58	664.98	10.98959	58	672.47	40.12207
59	686.44	63.88665	59	679.95	95.43441	59	686.10	66.65291
60	710.86	115.80905	60	708.93	113.69887	60	710.81	115.98240
61	737.38	255.87983	61	735.06	254.98125	61	737.37	256.44697
62	753.07	19.16228	62	751.75	17.75499	62	752.59	19.96765
63	757.03	58.97115	63	755.23	61.83872	63	756.91	57.64916
64	773.95	36.71039	64	772.05	39.45801	64	773.84	36.10247
65	792.45	77.27069	65	790.60	72.39280	65	792.19	77.52997
66	821.87	252.68911	66	818.93	248.36040	66	821.82	251.76266
67	831.05	75.84462	67	829.15	65.64481	67	831.04	75.98804
68	840.36	321.35981	68	837.08	316.72687	68	840.25	320.30384
69	863.25	34.42764	69	859.95	35.68113	69	863.12	34.32060
70	900.48	12.94661	70	877.73	9.34943	70	900.18	12.11854
71	933.96	147.02254	71	932.95	147.27235	71	931.33	152.58700
72	1016.26	48.51397	72	1014.44	47.77878	72	1016.26	48.53032
73	1052.61	13.19548	73	1051.41	11.75664	73	1048.01	12.90844
74	1060.51	113.59240	74	1058.30	115.09679	74	1060.50	112.95385
75	1101.55	136.35462	75	1099.35	135.71218	75	1098.48	5.69908
76	1108.54	18.27678	76	1106.64	17.75044	76	1101.74	145.37448
77	1137.72	135.21229	77	1134.34	137.40805	77	1137.66	135.45173
78	1198.01	14.25814	78	1195.59	19.82188	78	1196.28	12.61050
79	1288.97	39.63119	79	1284.99	104.69734	79	1286.48	33.73798
80	1320.80	218.25642	80	1306.41	160.16979	80	1319.02	222.58756
81	1451.61	103.36554	81	1447.61	82.99562	81	1450.52	105.63817
82	1505.31	9.44470	82	1505.12	10.03918	82	1505.18	9.53968
83	1553.33	6.79635	83	1547.02	8.70796	83	1553.29	6.80785
84	1626.36	89.68543	84	1625.51	99.84933	84	1622.59	87.48382
85	1670.54	155.91869	85	1664.07	157.02004	85	1670.54	155.97354
86	1679.15	66.61638	86	1672.93	65.74854	86	1679.15	66.53344
87	1684.00	57.71458	87	1677.72	57.19414	87	1684.00	57.70302
88	1697.54	89.82499	88	1691.27	96.63537	88	1697.54	89.94467
89	1701.12	25.79488	89	1694.98	25.36095	89	1701.12	25.79639
90	1705.51	52.32819	90	1699.21	51.16479	90	1705.51	52.34952
91	1712.48	62.33262	91	1706.24	61.22982	91	1712.48	62.37223
92	1728.09	30.14157	92	1721.79	32.08440	92	1728.09	30.12140
93	1746.00	44.85868	93	1737.46	84.09382	93	1745.99	44.88843

Continued on next page...

Table 126: Harmonic frequencies for the structure gw10-42, the global non–dissociated minimum of Gly•$(H_2O)_{10}$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number	IR intensity	mode	wave number	IR intensity	mode	wave number	IR intensity
	cm^{-1}	km/mol		cm^{-1}	km/mol		cm^{-1}	km/mol
94	1750.70	1.85818	94	1743.00	6.87858	94	1750.69	1.85566
95	1780.84	267.59785	95	1757.75	192.13470	95	1780.79	268.45096
96	2632.55	2108.45882	96	2622.25	2095.44134	96	2632.54	2108.52819
97	2992.49	1616.74369	97	2982.26	1608.43627	97	2992.49	1616.75702
98	3055.21	28.56274	98	3055.19	27.59029	98	3055.21	28.57246
99	3155.52	1.65893	99	3155.52	1.27772	99	3155.51	1.65930
100	3176.13	1321.73494	100	3165.58	1316.20351	100	3176.13	1321.73860
101	3262.63	997.42794	101	3252.07	991.86336	101	3262.63	997.42900
102	3458.80	355.09695	102	3448.17	350.84624	102	3458.80	355.15743
103	3479.17	459.07935	103	3471.13	470.54579	103	3479.15	458.47424
104	3509.93	494.85700	104	3496.62	576.25593	104	3509.11	477.29001
105	3519.07	1078.14356	105	3508.69	1058.79267	105	3519.00	1025.50623
106	3535.02	129.16555	106	3533.62	49.74573	106	3530.82	199.78783
107	3587.58	418.95080	107	3579.22	422.21418	107	3587.58	418.94922
108	3632.71	20.06275	108	3625.67	431.98428	108	3622.74	19.87453
109	3638.94	360.58315	109	3632.71	20.62630	109	3638.94	360.52001
110	3657.06	238.48283	110	3648.09	186.61882	110	3657.06	238.39778
111	3660.48	539.58512	111	3651.10	502.58251	111	3660.48	539.50023
112	3685.35	236.31756	112	3675.10	256.38502	112	3685.35	236.34335
113	3714.64	372.93404	113	3699.59	379.05180	113	3714.64	372.93309
114	3759.52	602.63609	114	3746.67	590.53156	114	3759.52	602.63310
115	3770.82	354.63659	115	3756.95	336.09663	115	3770.82	354.60811
116	3803.75	406.29156	116	3790.23	392.86038	116	3803.75	406.30437
117	3898.97	61.33834	117	3886.54	58.83549	117	3898.97	61.33842
118	3909.71	73.93307	118	3897.02	70.75021	118	3909.71	73.93290
119	3911.25	77.35063	119	3898.61	73.19206	119	3911.25	77.35075
120	3912.66	90.69989	120	3899.70	85.76146	120	3912.66	90.70070

Table 127: Harmonic frequencies for the structure gw10-68, the global zwitterionic minimum of Gly•$(H_2O)_{10}$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number	IR intensity	mode	wave number	IR intensity	mode	wave number	IR intensity
	cm^{-1}	km/mol		cm^{-1}	km/mol		cm^{-1}	km/mol
1	0.00	0.00000	1	-0.00	0.00000	1	-0.00	0.00000
2	0.00	0.00000	2	-0.00	0.00000	2	-0.00	0.00000
3	0.00	0.00000	3	-0.00	0.00000	3	-0.00	0.00000
4	0.00	0.00000	4	-0.00	0.00000	4	-0.00	0.00000
5	0.00	0.00000	5	-0.00	0.00000	5	0.00	0.00000
6	0.00	0.00000	6	0.00	0.00000	6	0.00	0.00000
7	30.55	1.65534	7	29.12	1.46192	7	30.51	1.66286
8	39.60	2.43192	8	37.86	2.28732	8	39.52	2.40180

Continued on next page...

Table 127: Harmonic frequencies for the structure gw10-68, the global zwitterionic minimum of Gly•$(H_2O)_{10}$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number	IR intensity	mode	wave number	IR intensity	mode	wave number	IR intensity
	cm^{-1}	km/mol		cm^{-1}	km/mol		cm^{-1}	km/mol
9	47.44	0.24913	9	45.27	0.20457	9	47.39	0.25354
10	52.56	3.71197	10	49.96	3.29914	10	52.55	3.72146
11	55.87	0.20400	11	53.06	0.17789	11	55.85	0.20586
12	59.74	0.44227	12	56.97	0.40573	12	59.61	0.43442
13	66.98	1.39559	13	64.00	1.24055	13	66.81	1.42025
14	75.09	2.60946	14	71.40	2.77812	14	75.02	2.55335
15	75.63	1.85357	15	71.86	1.35171	15	75.62	1.82149
16	78.99	3.33558	16	75.00	2.93412	16	78.97	3.39508
17	81.82	0.36347	17	77.89	0.33480	17	81.78	0.37842
18	92.87	3.59967	18	89.32	3.26621	18	92.37	3.54549
19	103.59	1.12808	19	98.12	1.07012	19	103.58	1.12370
20	135.20	0.59129	20	128.65	0.60504	20	135.18	0.58615
21	145.53	14.08377	21	141.01	14.73150	21	145.48	13.93901
22	159.66	4.48309	22	154.24	1.87599	22	159.17	4.73658
23	166.59	2.41342	23	159.05	2.29846	23	166.52	2.37521
24	176.39	3.91985	24	167.88	3.62802	24	176.31	3.84997
25	184.05	2.94524	25	174.93	2.28499	25	184.05	2.95647
26	192.71	2.59226	26	183.04	2.47463	26	192.68	2.55389
27	201.45	8.79452	27	191.67	7.52398	27	201.29	9.03909
28	206.85	18.32867	28	196.78	17.68988	28	206.70	18.13631
29	215.07	0.52931	29	204.96	0.86212	29	214.96	0.53479
30	219.17	15.02121	30	208.35	14.74075	30	219.08	14.61975
31	238.08	32.43336	31	227.66	31.48051	31	237.32	35.23142
32	248.22	60.13310	32	245.80	31.87522	32	248.12	58.29234
33	255.68	112.24172	33	247.65	37.40244	33	255.52	103.64056
34	258.93	47.64805	34	253.87	150.44868	34	258.49	54.27351
35	266.42	44.40445	35	256.95	31.20168	35	264.67	44.60336
36	283.83	43.89480	36	276.14	14.40168	36	283.80	43.47362
37	289.57	27.61083	37	279.44	63.83848	37	289.49	26.62247
38	304.44	17.63295	38	295.77	4.45892	38	304.43	17.65856
39	310.82	26.12934	39	302.45	28.24373	39	310.80	25.68923
40	328.97	65.84667	40	326.00	59.27391	40	328.97	65.80517
41	347.31	24.17322	41	331.15	19.92398	41	346.60	31.11824
42	353.96	34.60193	42	337.30	35.24440	42	353.70	33.33351
43	367.54	128.45121	43	359.78	125.37111	43	364.02	120.15962
44	415.71	89.63713	44	414.63	90.43569	44	415.68	88.95852
45	461.63	64.98940	45	459.71	77.21069	45	461.45	67.83861
46	468.40	40.23543	46	466.87	41.82152	46	467.89	38.68519
47	484.64	45.47961	47	481.68	32.44681	47	484.25	44.64095
48	504.22	25.39956	48	495.98	38.69998	48	502.82	26.23485
49	514.92	6.48488	49	511.53	7.37931	49	513.73	7.20814
50	527.66	17.14475	50	525.52	16.31514	50	527.40	16.03016
51	557.05	30.65671	51	554.86	29.51854	51	557.03	30.71914
52	571.74	29.43836	52	570.04	30.38224	52	571.62	29.12434
53	577.18	31.44290	53	575.73	30.63910	53	577.13	31.46038
54	603.69	50.95561	54	595.98	41.17217	54	603.21	47.46297
55	612.85	66.77505	55	609.99	74.47962	55	612.67	67.82799

Continued on next page...

Table 127: Harmonic frequencies for the structure gw10-68, the global zwitterionic minimum of Gly•$(H_2O)_{10}$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol
56	637.99	53.69173	56	637.04	52.64218	56	637.94	54.11335
57	655.65	34.80800	57	653.99	33.59383	57	655.63	34.97976
58	679.09	41.41933	58	676.24	61.65409	58	679.06	41.85508
59	690.20	141.28239	59	683.08	45.78155	59	690.10	140.27470
60	697.66	66.85414	60	694.93	80.32972	60	697.61	66.42402
61	705.10	6.38581	61	696.10	65.23637	61	704.77	6.88621
62	734.26	191.76309	62	731.23	194.15145	62	734.26	191.76599
63	768.54	186.96683	63	766.38	182.64091	63	768.53	187.01883
64	802.47	196.31537	64	799.77	195.87364	64	802.44	196.56834
65	818.44	276.55005	65	815.30	279.94721	65	818.37	277.14184
66	848.87	71.51758	66	846.18	70.26613	66	848.80	71.21891
67	875.24	195.41028	67	872.85	189.07531	67	875.23	195.47678
68	881.28	80.76319	68	875.95	45.48121	68	881.16	80.18161
69	906.22	69.06293	69	892.19	62.09049	69	906.16	68.50068
70	913.89	42.20022	70	904.67	73.83554	70	913.30	44.72233
71	956.89	120.24787	71	954.86	129.10185	71	956.82	122.21782
72	959.56	19.57573	72	956.87	3.45205	72	959.47	17.74182
73	1016.74	37.53865	73	1014.68	37.46527	73	1016.65	37.40517
74	1055.85	58.25411	74	1054.15	72.55225	74	1045.40	9.48582
75	1058.72	79.35532	75	1056.79	63.96464	75	1057.45	128.46695
76	1143.16	10.67647	76	1142.19	11.51836	76	1142.03	11.72918
77	1186.73	48.87507	77	1186.13	49.05911	77	1183.13	52.12843
78	1358.62	28.01708	78	1348.57	128.73835	78	1352.93	22.70638
79	1363.69	75.15406	79	1358.92	17.09358	79	1361.54	78.55131
80	1427.82	146.23745	80	1410.62	97.79149	80	1427.02	148.46358
81	1496.92	5.92282	81	1496.40	9.73312	81	1496.51	7.35624
82	1527.74	149.25446	82	1526.76	156.72731	82	1522.29	146.19168
83	1651.98	111.75399	83	1645.91	213.32862	83	1651.45	111.81129
84	1656.70	95.65723	84	1650.02	104.24771	84	1656.65	95.01146
85	1672.38	239.32419	85	1665.38	257.32887	85	1672.36	240.78135
86	1683.87	95.51596	86	1674.64	69.27704	86	1683.85	94.81263
87	1688.30	95.67068	87	1681.14	93.89288	87	1688.16	96.06053
88	1703.34	137.59764	88	1693.80	73.48282	88	1703.31	139.43850
89	1708.34	19.92484	89	1701.61	7.54189	89	1708.33	18.72955
90	1710.03	133.29407	90	1703.08	95.69655	90	1709.92	133.29946
91	1722.44	68.11406	91	1716.17	68.52481	91	1722.44	68.17231
92	1727.95	27.50822	92	1722.06	21.97283	92	1727.95	27.19834
93	1739.41	14.07994	93	1737.62	22.88524	93	1738.12	15.57578
94	1744.60	41.49993	94	1739.27	23.40162	94	1744.58	41.07703
95	1753.68	50.15999	95	1747.47	33.72794	95	1753.68	50.09106
96	3073.71	479.53922	96	3071.88	506.54956	96	3068.38	496.14191
97	3105.81	1146.39431	97	3096.16	1100.38915	97	3105.39	1144.35304
98	3143.81	26.86247	98	3140.31	867.64762	98	3143.68	30.09072
99	3151.08	921.59700	99	3144.11	95.11828	99	3150.98	909.04272
100	3186.48	1010.87165	100	3185.84	1025.45858	100	3179.61	975.47338
101	3216.17	9.11500	101	3216.16	9.58437	101	3216.12	5.89111
102	3246.20	881.77272	102	3236.65	857.18394	102	3245.56	924.04353

Continued on next page...

Table 127: Harmonic frequencies for the structure gw10-68, the global zwitterionic minimum of Gly•$(H_2O)_{10}$ computed at the SCS-MP2/TZVPP level of theory. Natural isotopes as well as the isotopic substitutions $^{16}O \rightarrow ^{18}O$ and $^{14}N \rightarrow ^{15}N$ are included.

Bare spectrum			$^{16}O \rightarrow ^{18}O$			$^{14}N \rightarrow ^{15}N$		
mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol	mode	wave number cm^{-1}	IR intensity km/mol
103	3307.65	1188.50430	103	3296.96	1179.07094	103	3307.63	1191.81488
104	3402.31	959.31541	104	3392.53	962.35805	104	3401.88	950.81144
105	3444.93	192.01728	105	3444.69	192.43538	105	3437.14	184.71564
106	3523.32	522.59671	106	3512.63	514.61061	106	3523.32	522.32823
107	3552.48	85.44963	107	3541.13	68.58658	107	3552.47	86.08507
108	3556.19	677.94943	108	3545.79	717.20129	108	3556.18	677.83475
109	3597.96	648.19843	109	3587.80	625.28159	109	3597.92	648.58455
110	3631.62	581.59720	110	3622.29	585.56959	110	3631.62	581.49962
111	3635.86	180.03336	111	3625.68	231.42626	111	3635.85	179.90882
112	3654.12	399.54542	112	3642.96	349.14792	112	3654.12	399.80247
113	3699.62	529.80212	113	3684.75	531.13832	113	3699.62	529.75387
114	3736.13	442.16648	114	3722.26	435.78561	114	3736.13	442.11390
115	3745.71	466.46042	115	3733.20	441.23802	115	3745.71	466.45991
116	3901.34	72.32565	116	3888.82	69.08426	116	3901.34	72.32427
117	3908.92	69.94919	117	3896.31	66.17300	117	3908.92	69.95156
118	3917.51	87.80827	118	3904.73	82.21461	118	3917.51	87.82314
119	3924.25	86.92047	119	3911.31	82.14061	119	3924.25	86.99285
120	3927.44	105.91146	120	3914.05	99.25370	120	3927.44	105.93043

Table 128: Masses of different isotopes used for hydrogen, carbon, nitrogen and oxygen. Data taken from The National Institute of Standards and Technology (NIST).

Element	A	mass (u)
H	1	1.007825
	2	2.014100
C	12	12.000000
	13	13.003355
N	14	14.003074
	15	15.000108
O	16	15.994915
	18	17.999160

References

(1) CP2k Developers Team, http://www.cp2k.org.

(2) Aikens, C. M.; Gordon, M. S. Incremental Solvation of Nonionized and Zwitterionic Glycine. *J. Am. Chem. Soc.* **2006**, *128*, 12835–12850.

(3) Kayi, H.; Kaiser, R. I.; Head, J. D. A theoretical investigation of the relative stability of hydrated glycine and methylcarbamic acid–from water clusters to interstellar ices. *Phys. Chem. Chem. Phys.* **2012**, *14*, 4942–4958.

(4) TURBOMOLE V6.2 2010, a development of University of Karlsruhe and Forschungszentrum Karlsruhe GmbH, 1989-2007, TURBOMOLE GmbH. `http://www.turbomole.com`. (2007).