Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Hydrogen Bond Mediated Stabilization of the Salt Bridge Structure for the Glycine Dimer Anion

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Supporting Information

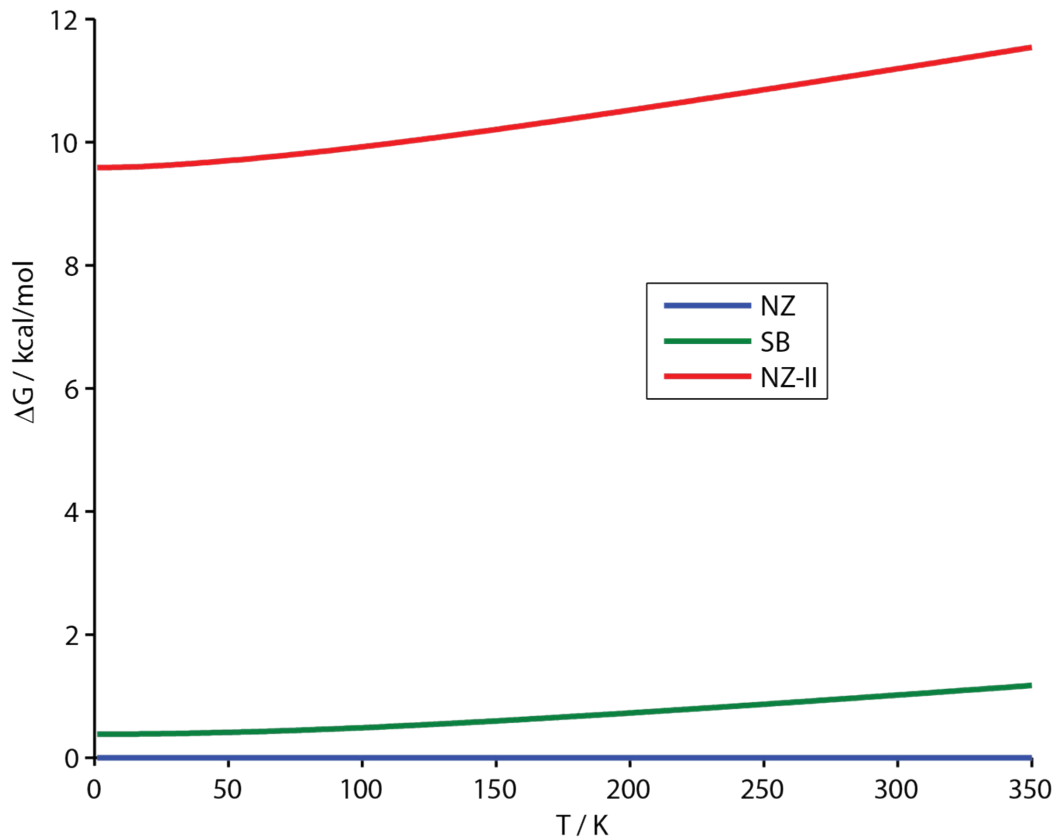

Figure S1. ΔG in kcal/mol for the isomers NZ, SB and NZ-II at the B3LYP/6-311++G** level of theory with respect to NZ as a function of temperature.

Table S1. Comparison of the most intense experimental IRMPD transitions with the B3LYP/6-311++G** most intense predicted harmonic vibrations scaled by 0.985 for $[Gly_2\text{-}H]^-$ and the possible peak assignment.

Experiment / cm^{-1}	Vibration (SB)	Wavenumber / cm^{-1}	Vibration (NZ)	Wavenumber / cm^{-1}
1704	"Free" ν_{asymm}	1697	ν_{asymm} COOH	1782
1622	NH_3^+ stretch, ν_{asymm}, NH_3^+ umbrella	1624, 1579, 1508	ν_{asymm} COO^-	1685
			H−O bending	1496
1404	ν_{symm}	1379	ν_{symm} COO^-	1397
1345	"Free" ν_{symm}	1316	ν_{symm} COOH	1339
1000-1300	NH_3^+, NH_2, CH_2 wagging	1146	O···H−O stretch	1157, 1137, 1091

			combined with NH_2, CH_2 wagging	
940	NH_2, CH_2 wagging	962	NH_2, CH_2 wagging	955
835	NH_2, CH_2 wagging, NH_3^+, CH_2 wagging	865, 842	NH_2, CH_2 wagging	847

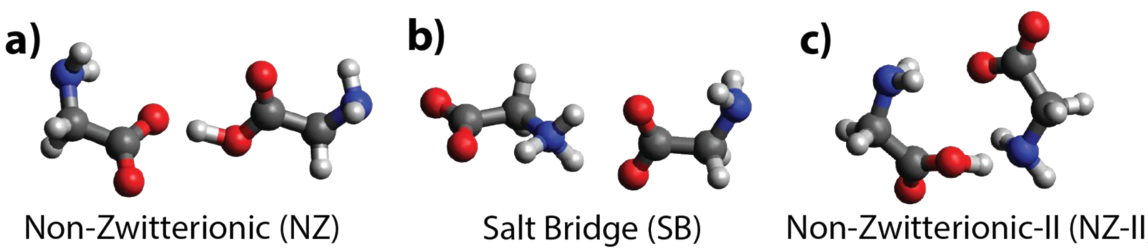

Figure S2. Structural isomers for $[Gly_2\text{-}H]^-$ with non-zwitterionic (NZ + NZ-II) a)+c) and salt bridge (SB) structure b) computed at the B3LYP/6-311++G** level of theory. Oxygen, nitrogen, carbon and hydrogen atoms are represented by red, blue, gray and white spheres, respectively.

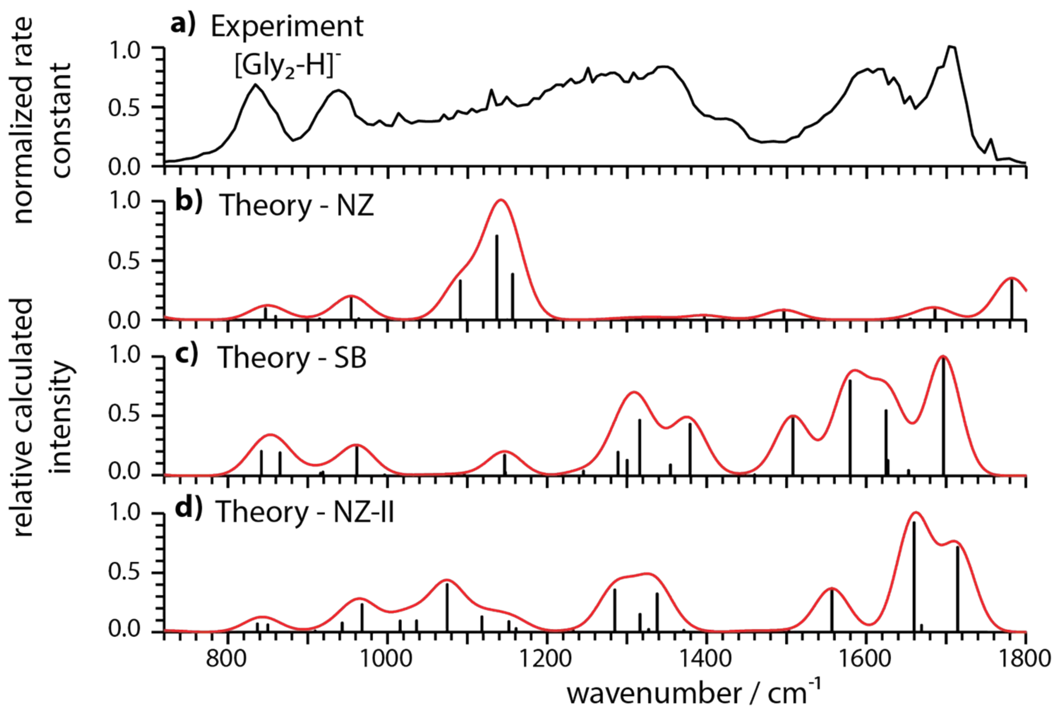

Figure S3. Comparison of the a) experimental IRMPD spectrum of $[Gly_2\text{-}H]^-$ with the harmonic vibrational spectra for b) NZ, c) SB and d) NZ-II. The theoretical IR spectra were computed employing the B3LYP/6-311++G** level of theory and using a uniform scaling factor of 0.985.

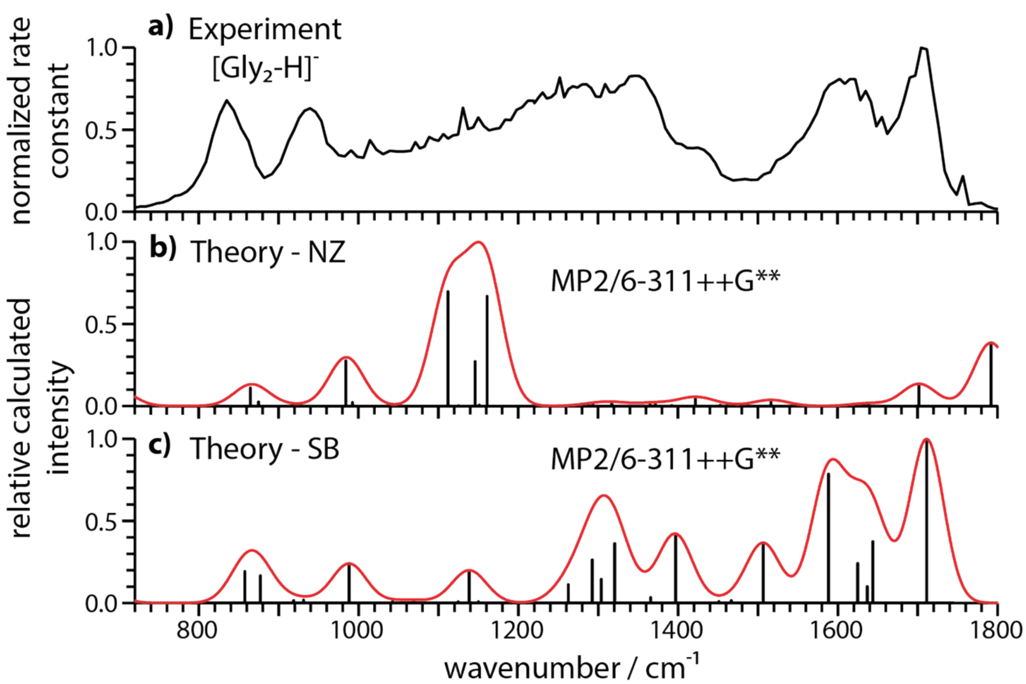

Figure S4. Comparison of the a) experimental IRMPD spectrum of $[Gly_2\text{-}H]^-$ with the harmonic vibrational spectra for b) NZ and c) SB. The theoretical IR spectra were computed employing the MP2/6-311++G** level of theory and using a uniform scaling factor of 0.980.

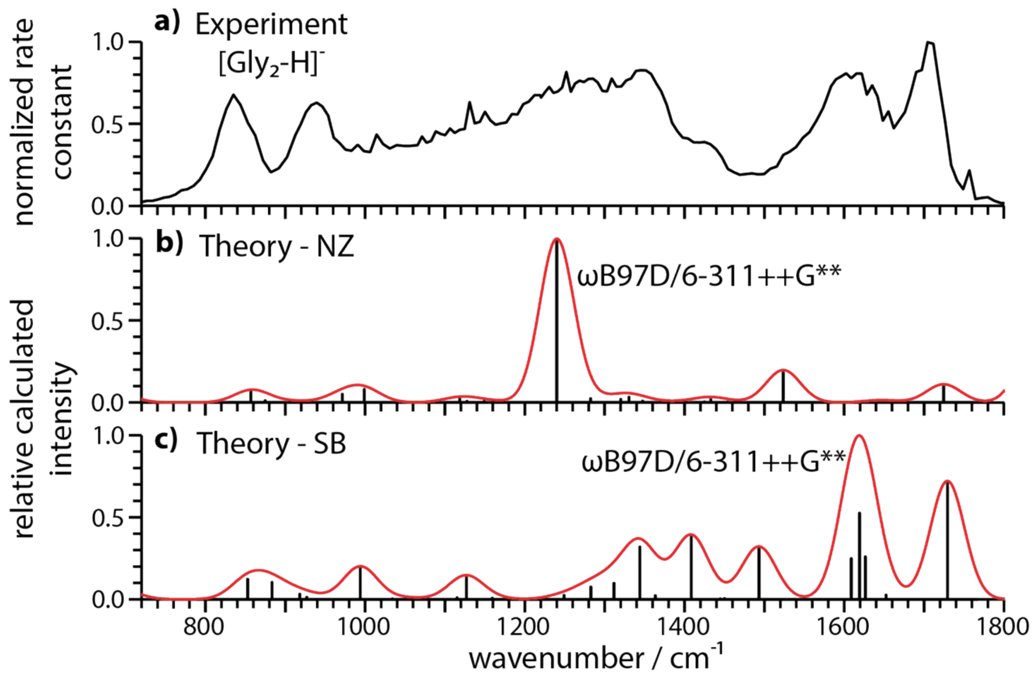

Figure S5. Comparison of the a) experimental IRMPD spectrum of $[Gly_2\text{-}H]^-$ with the harmonic vibrational spectra for b) NZ and c) SB. The theoretical IR spectra were computed employing the ωB97D/6-311++G** level of theory and using a uniform scaling factor of 0.975.

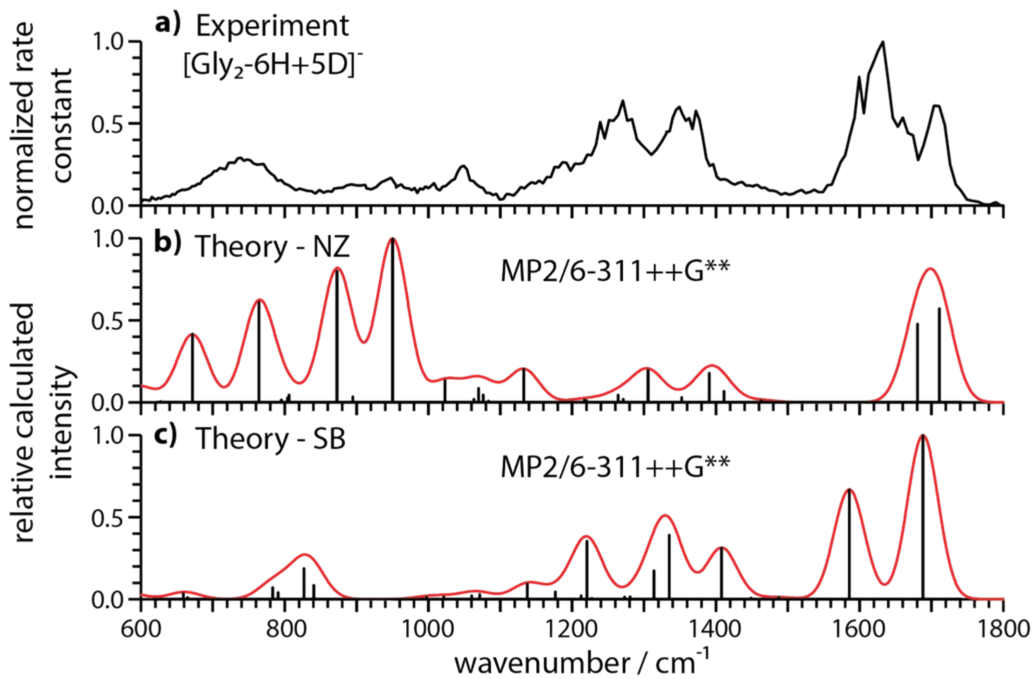

Figure S6. Comparison of the a) experimental IRMPD spectrum of $[Gly_2\text{-}6H+5D]^-$ with the harmonic vibrational spectra for b) NZ and c) SB. The theoretical IR spectra were computed employing the MP2/6-311++G** level of theory and using a uniform scaling factor of 0.980.

Table S2. Comparison of the most intense experimental IRMPD transitions with the B3LYP/6-311++G** most intense predicted harmonic vibrations scaled by 0.985 for $[Gly_2\text{-}6H+5D]^-$ and a possible peak assignment.

Experiment / cm^{-1}	Vibration (SB)	Wavenumber / cm^{-1}	Vibration (NZ)	Wavenumber / cm^{-1}
1703	"Free" $\nu_{antisymm}$	1688	$\nu_{antisymm}$ COOH	1710
1632	$\nu_{antisymm}$	1579	$\nu_{antisymm}$ COO^-	1676
1484-1401	ν_{symm}	1382		
1349	"Free" ν_{symm}	1320	NH_2, CH_2 wagging, ν_{symm} COO^-	1360
1270	NH_3^+ stretch	1196	NH_2, CH_2 wagging, ν_{symm} COOH	1285
1198-1104	NH_3^+ umbrella	1130	H−O bending	1135
1049	N−C sretch	1038	NH_2, CH_2 wagging	1048
948	N−C sretch	972	O···H−O stretch	946

739	NH_3^+, NH_2, CH_2 wagging	819, 800, 776, 749	NH_2, CH_2 wagging and O···H−O stretch	868, 752, 652

xyz coordinates at the B3LYP/6-311++G level of theory**

[Gly$_2$-2H+Na]$^-$

7	4.867234442	-0.918239369	0.388686134
6	4.187188515	0.215587824	-0.252645961
6	2.644791335	0.223440453	-0.166279568
8	2.035675744	1.042619032	-0.905031770
8	2.100726437	-0.564975030	0.656217080
1	4.350920548	-1.117373841	1.244008677
1	4.533058420	1.147772642	0.209951755
1	4.477426853	0.274516517	-1.304798858
7	-4.867203313	-0.918338219	-0.388652195
6	-4.187203887	0.215645234	0.252454890
6	-2.644798933	0.223456361	0.166218951
8	-2.035734806	1.042821769	0.904807174
8	-2.100674917	-0.565182401	-0.656023786
1	-4.350794503	-1.117707015	-1.243862824
1	-4.533022026	1.147717069	-0.210408848
1	-4.477532781	0.274841422	1.304567535
11	0.000001852	0.278542750	0.000044446
1	4.716600024	-1.744693971	-0.184043161
1	-4.716647281	-1.744643891	0.184312868

NZ - [Gly$_2$-H]$^-$

6	2.164341650	0.586312683	0.116041486
8	1.990905489	1.692264322	0.636807223
8	1.295555868	-0.145285059	-0.484050314
1	4.032063171	0.192690994	1.114463139
1	4.183798625	0.576016131	-0.586186210
1	0.015776465	0.217274627	-0.545363141
6	3.595127548	-0.007082123	0.132724230
7	3.734602288	-1.434639832	-0.188455774
1	3.328379951	-1.970284674	0.574645907
1	3.108433367	-1.619418801	-0.969917118
6	-1.970988870	-0.148412660	-0.109604299
8	-1.826340468	-1.107232872	0.639025055
8	-1.042786333	0.517936366	-0.728953873
1	-3.561397049	0.169421598	-1.500554048
1	-3.378775969	1.467540361	-0.343540506
6	-3.380658712	0.379021789	-0.439913554

7	-4.468022880	-0.189487731	0.360455690
1	-4.407769222	0.189032892	1.301856380
1	-4.269389060	-1.181054133	0.478526564

SB - $[Gly_2\text{-}H]^-$

6	2.100968683	0.325909720	0.029901071
8	1.425175968	1.273636133	0.519387391
8	1.658228822	-0.657986947	-0.625450339
1	3.829937200	0.722645129	1.258517723
1	3.986866384	1.227288211	-0.408589837
1	-0.219863742	-0.455753304	-0.661046142
6	3.631857258	0.409752426	0.230334930
7	4.397650118	-0.804565123	-0.075864874
1	3.974752231	-1.216047309	-0.906133055
1	4.218922921	-1.488427442	0.654825340
6	-3.378093774	-0.146654887	0.004488681
8	-4.325742683	-0.602440664	0.658913803
8	-3.356743681	0.500480930	-1.077157234
1	-1.781807086	-1.484597510	0.700138397
1	-1.884045176	0.033270350	1.604884795
6	-1.953401367	-0.412305364	0.613087845
7	-0.936160372	0.197461573	-0.291553947
1	-0.297735692	0.898071435	0.150080811
1	-1.538105241	0.605371966	-1.042399275

NZ-II - $[Gly_2\text{-}H]^-$

6	-1.941279832	-0.486805350	0.063991252
8	-2.210727872	-1.305401544	-0.796535641
8	-1.106071822	-0.716154815	1.075890337
1	-3.205721370	1.030803748	0.902440058
1	-3.070419923	1.058200869	-0.857240822
1	-0.337825993	-1.324693951	0.748469745
6	-2.500987734	0.936890432	0.066967158
7	-1.494910566	1.994328783	0.173891432
1	-1.042596991	1.926398020	1.080892961
1	-0.739075015	1.819544781	-0.493043145
6	2.031938761	0.525574384	-0.202603555
8	1.150078806	0.667834379	-1.091801188
8	2.827209597	1.358315206	0.270566578
1	2.200911885	-0.848069219	1.474985059
1	3.124271472	-1.325252433	0.045102027
6	2.161986071	-0.921238452	0.385315153
7	1.023065907	-1.768283358	-0.031421299
1	0.739812265	-1.415717703	-0.950103621
1	1.273765641	-2.748266642	-0.113876855

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