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

Competition between Salt Bridge and Non-Zwitterionic Structure in Deprotonated Amino Acid Dimers

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Electronic Supporting Information

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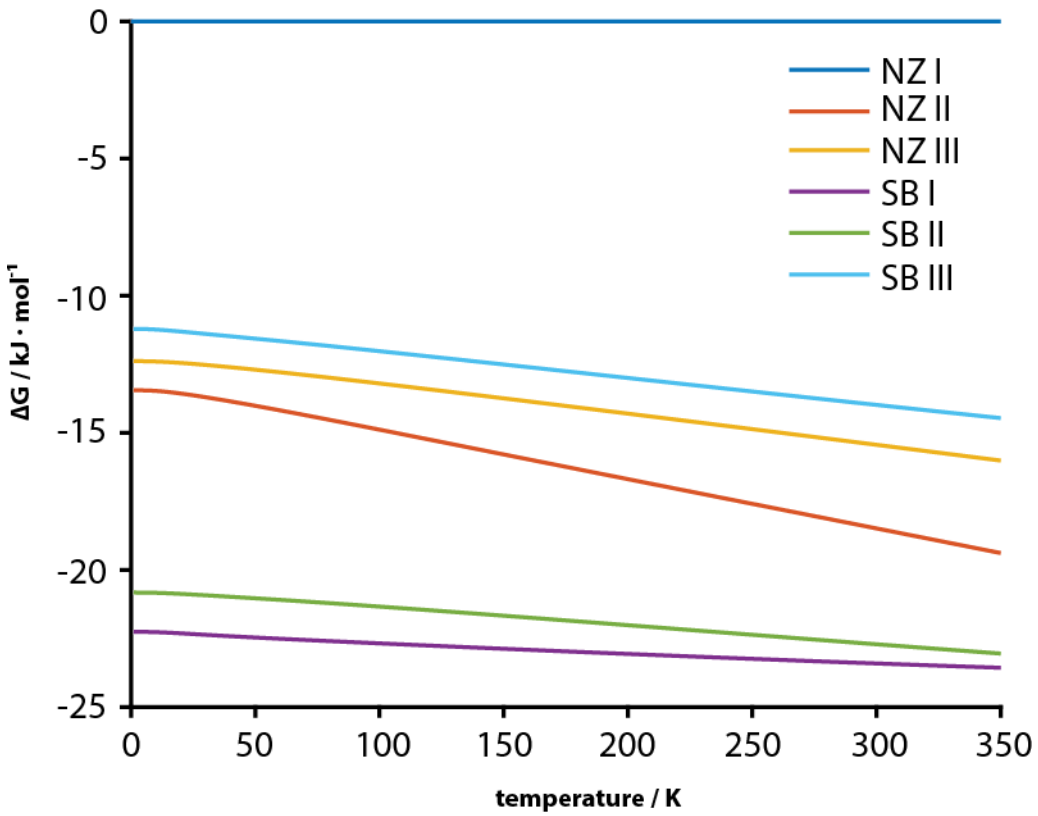

Figure S1. ΔG in kJ/mol for the isomers of $[2Pro-H]^-$ at the B3LYP/GCR level of theory with respect to NZ I as a function of temperature.

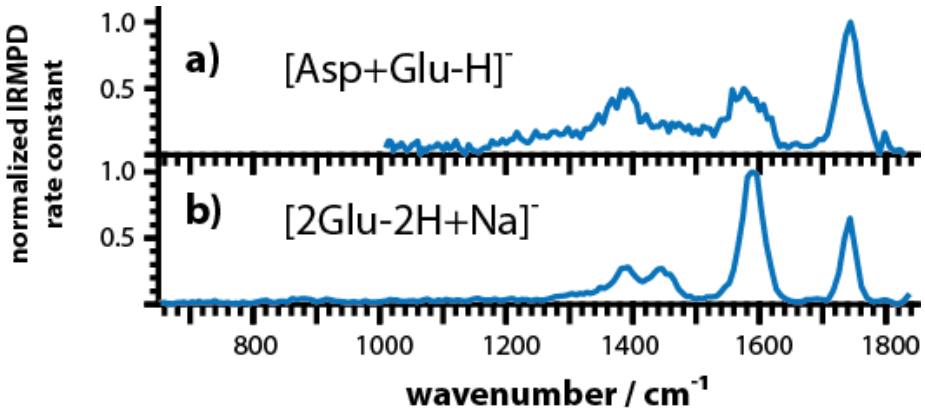

Figure S2. IRMPD spectra of (a) $[Asp+Glu-H]^-$ and (b) $[2Glu-2H+Na]^-$ at 298 K.

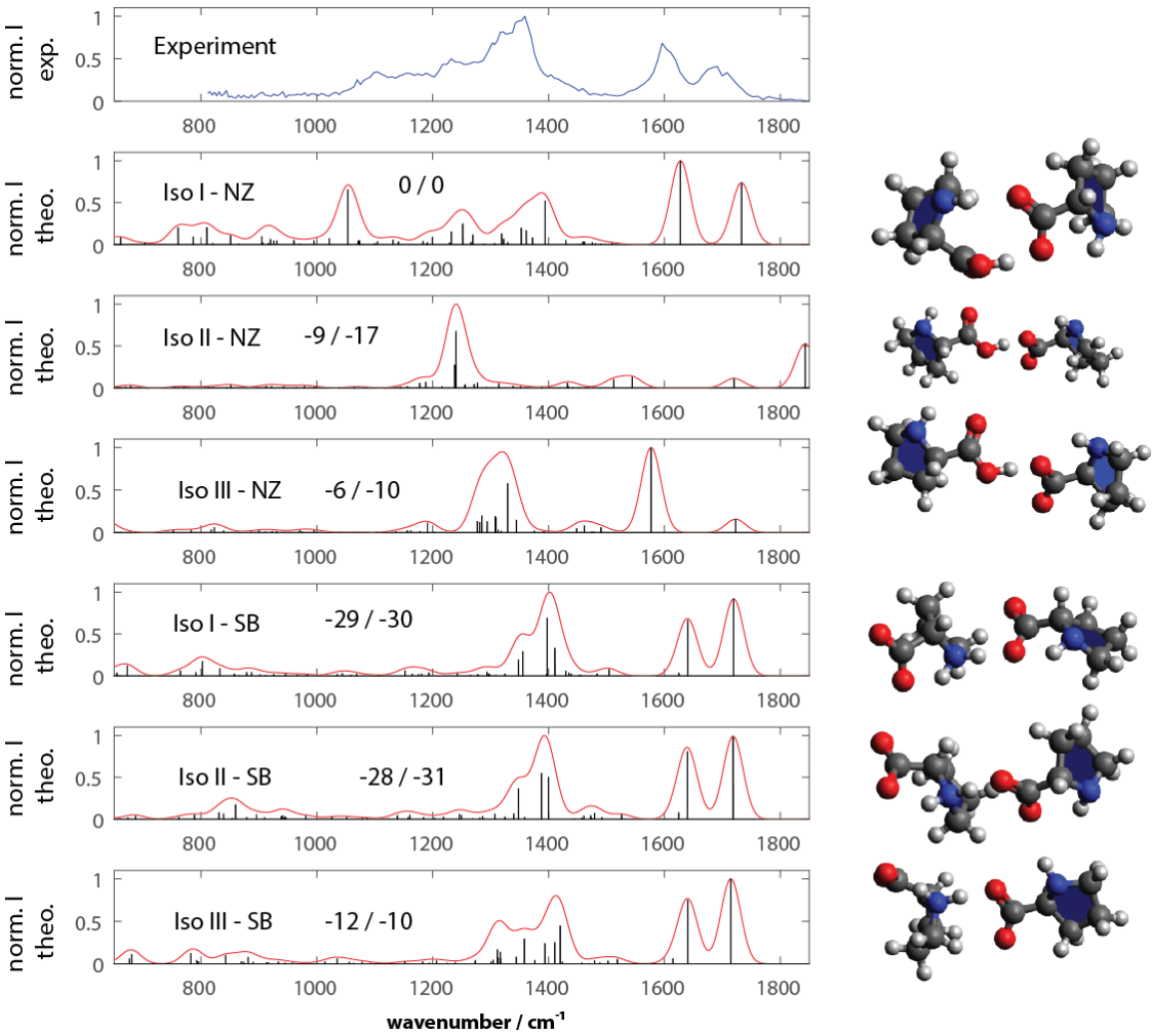

Figure S3. Comparison between experiment and theory for $[2Pro\text{-}H]^-$ at the ωB97-D/GCR level of theory. Harmonic frequencies were scaled with a uniform scaling factor of 0.975 and corresponding structures are shown to the right of every calculated spectrum.

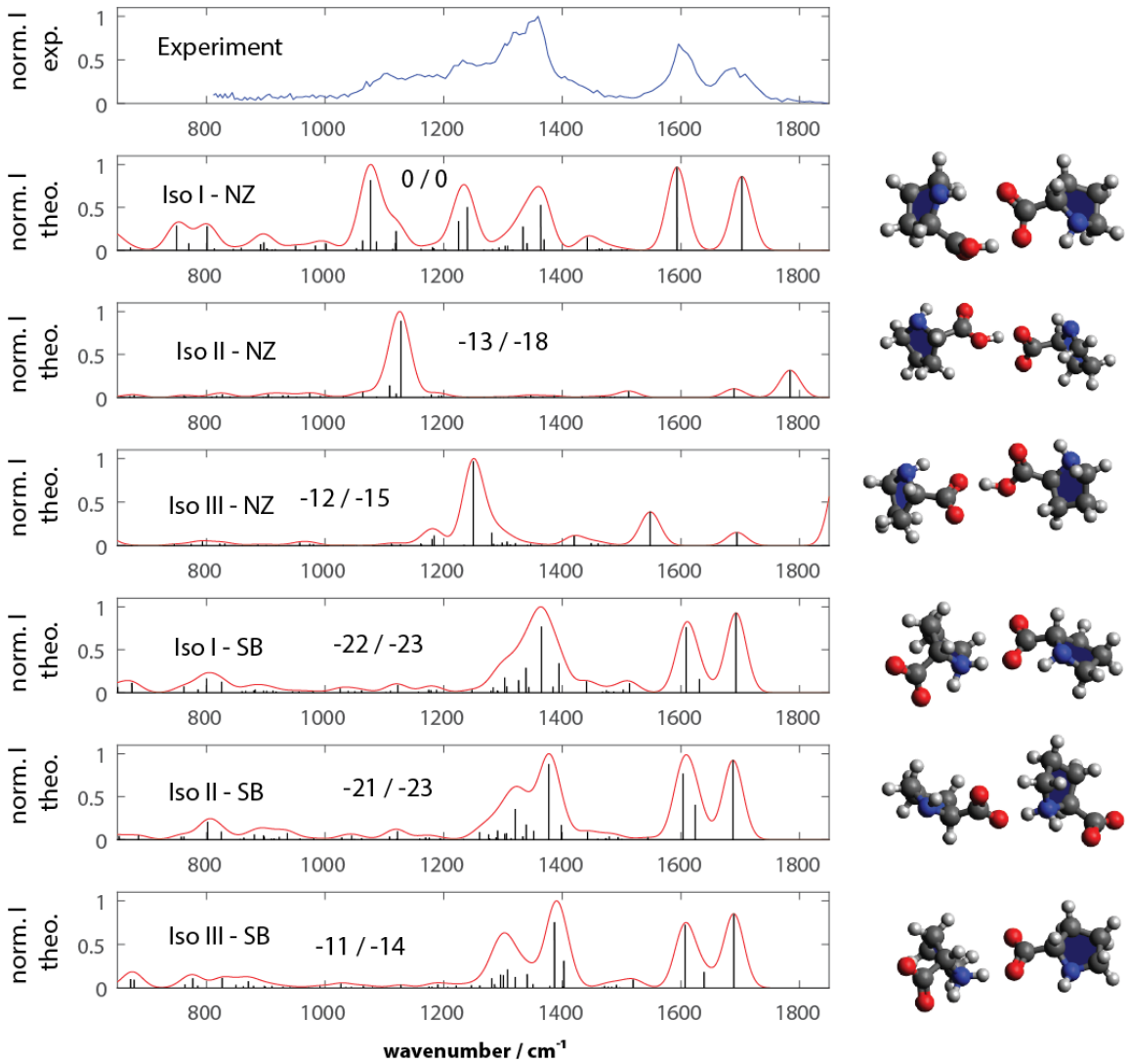

Figure S4. Comparison between experiment and theory for [2Pro-H]$^-$ at the B3LYP/GCR level of theory. Harmonic frequencies were scaled with a uniform scaling factor of 0.987 and corresponding structures are shown to the right of every calculated spectrum.

Table S1. Relative Gibbs free energy difference of the SB isomer of some negative amino acid dimer with respect to NZ structure at 0 and 298 K at different levels of theory (in kJ/mol).

Dimer	Level of theory	ΔG(0 K) / kJ/mol	ΔG(298 K) / kJ/mol
[2Cys-H]-	B3LYP/GCR	2	3
	ωB97-D/GCR	4	-5
[2Cys-3H]-	B3LYP/GCR	21	19
	ωB97-D/GCR	27	16
[2Glu-H]-	B3LYP/GCR	-2	1
	ωB97-D/GCR	-7	-9
[2Pro-H]-	B3LYP/GCR	-8	-5
	ωB97-D/GCR	-19	-14
	MP2/GCR//B3LYP/GCR	-16	-18
[2Phe-H]-	B3LYP/GCR	-13	-18
	ωB97-D/GCR	-4	-1

[2His-H]⁻	B3LYP/GCR	28	20

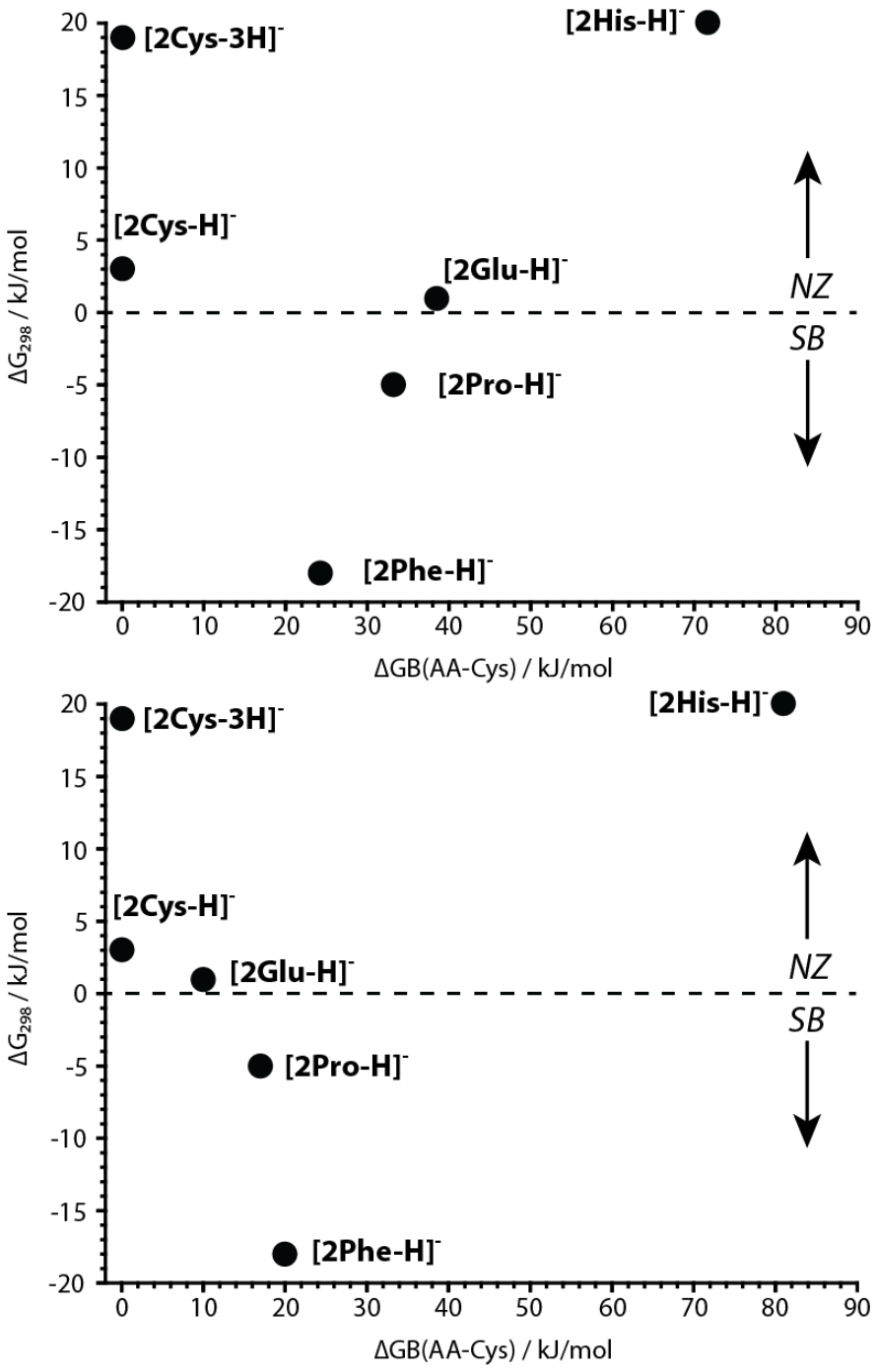

Figure S5. Gibbs free energy difference between NZ minus SB isomers of negative amino acid dimers at 298 K (ΔG_{298}) from B3LYP/GCR computations as a function of amino acid (AA = Cys, Glu, Pro, Phe, His) gas phase basicity difference relative to the cysteine gas phase basicity, ΔGB(AA-Cys).[1,2] For [2Cys-3H]$^-$ the GB value of Cys was used. In a) ΔGB(AA-Cys) values are taken from ref. 1 in b) from ref. 2.

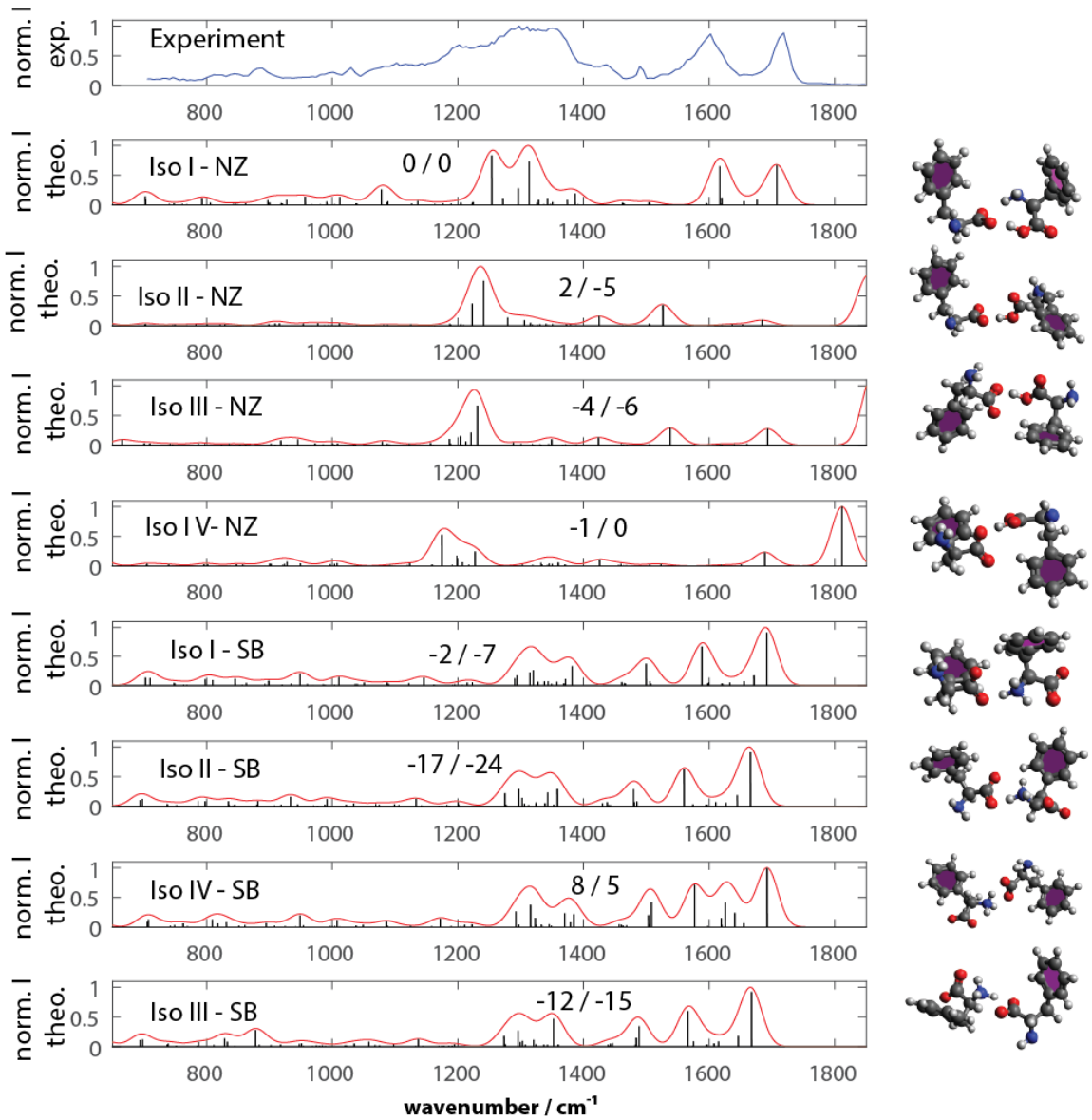

Figure S6. Comparison between experiment and theory for [2Phe-H]$^-$ at the B3LYP/GCR level of theory. Harmonic frequencies were scaled with a uniform scaling factor of 0.987 and corresponding structures are shown to the right of every calculated spectrum.

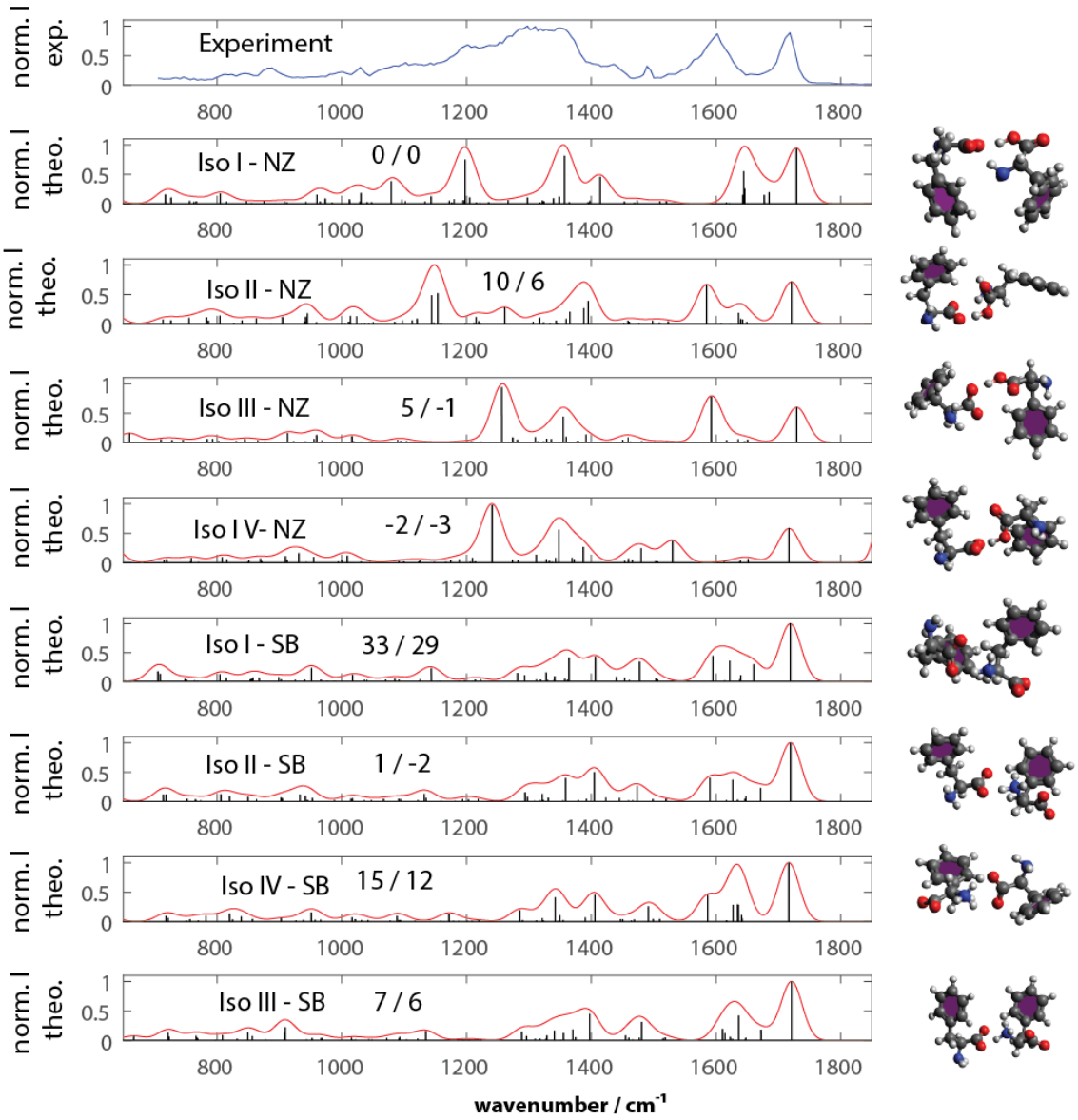

Figure S7. Comparison between experiment and theory for [2Phe-H]$^-$ at the ωB97-D/GCR level of theory. Harmonic frequencies were scaled with a uniform scaling factor of 0.975 and corresponding structures are shown to the right of every calculated spectrum.

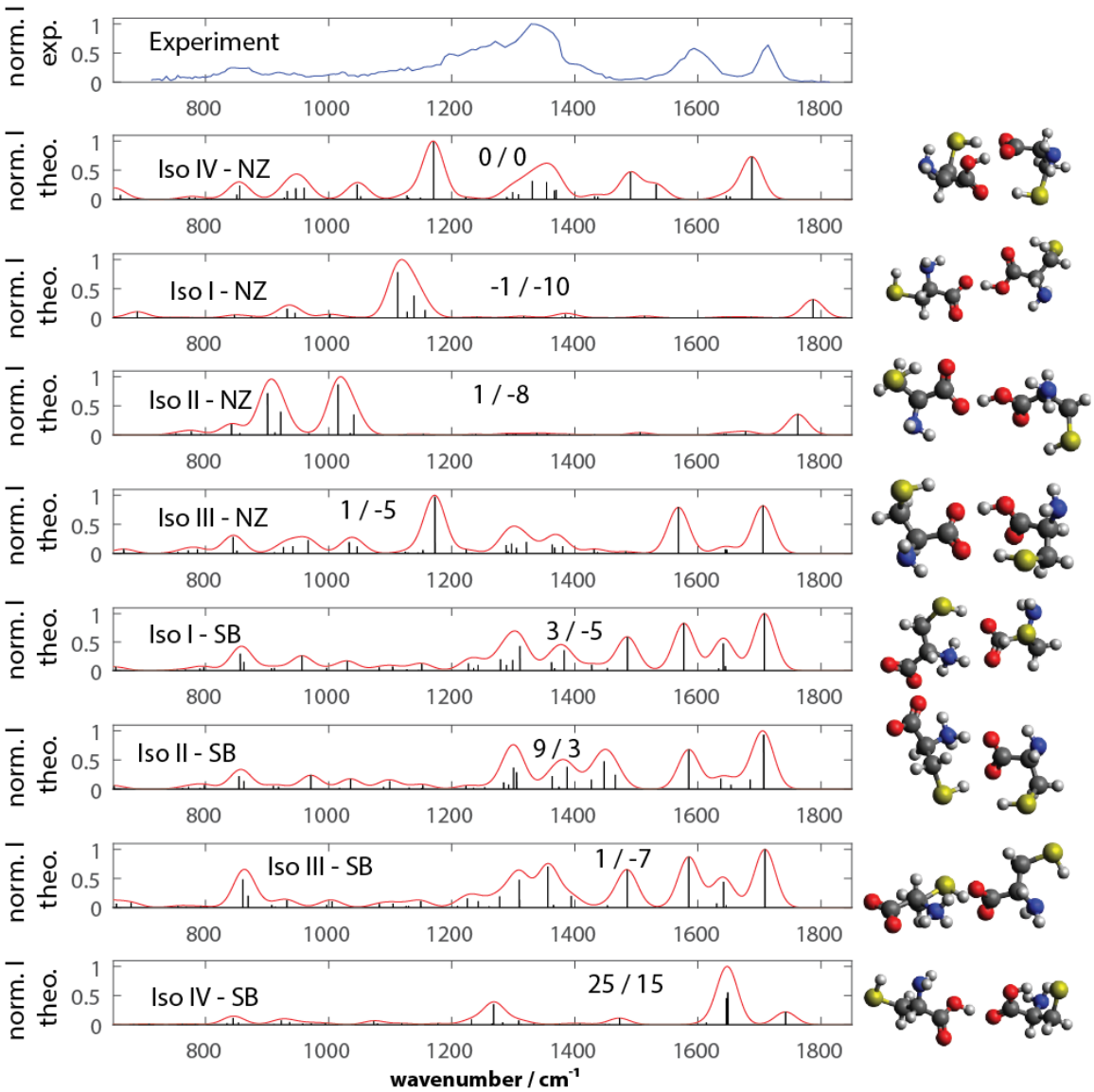

Figure S8. Comparison between experiment and theory for [2Cys-H]$^-$ at the B3LYP/GCR level of theory. Harmonic frequencies were scaled with a uniform scaling factor of 0.987 and corresponding structures are shown to the right of every calculated spectrum.

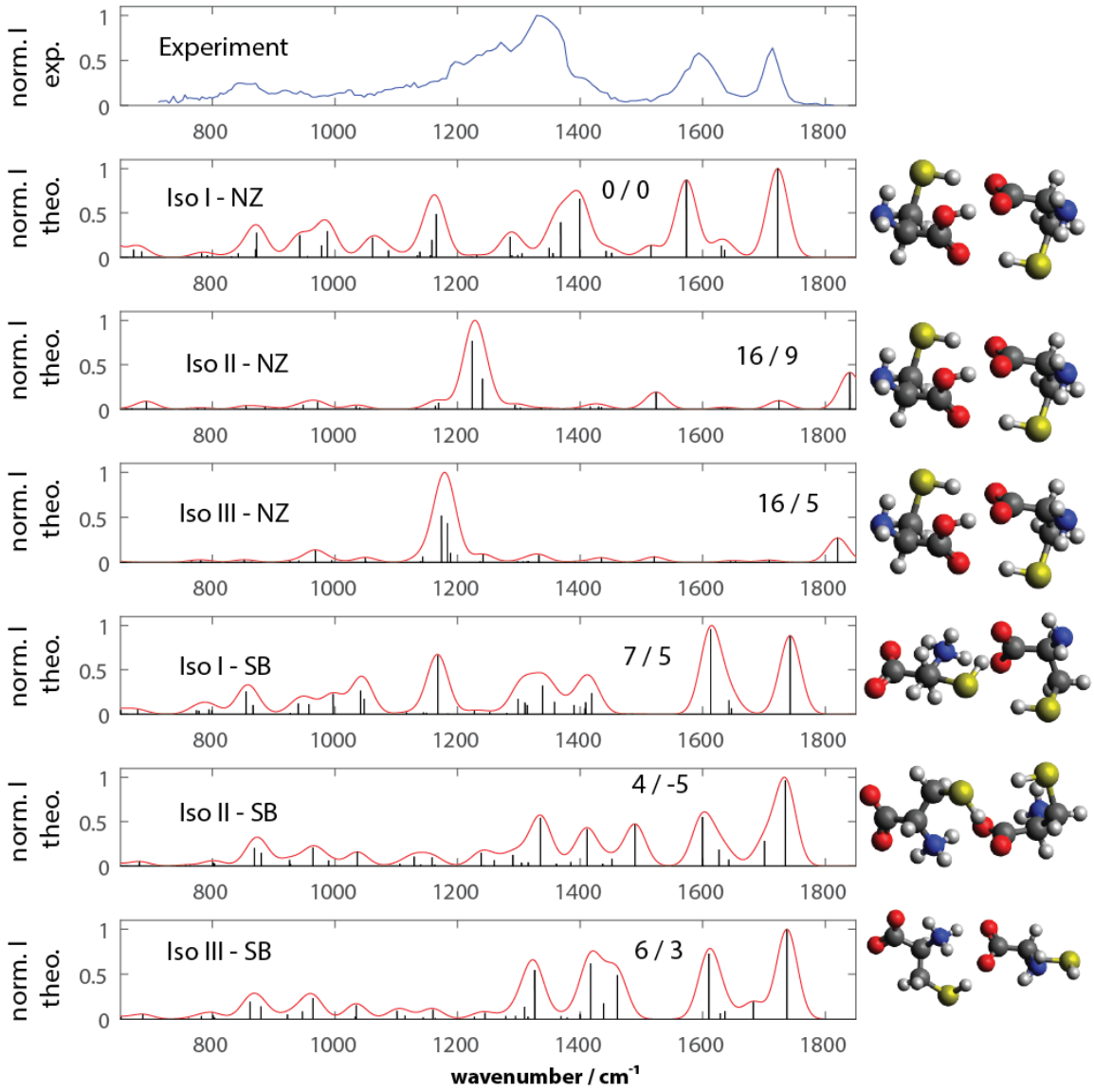

Figure S9. Comparison between experiment and theory for [2Cys-H]$^-$ at the ωB97-D/GCR level of theory. Harmonic frequencies were scaled with a uniform scaling factor of 0.975 and corresponding structures are shown to the right of every calculated spectrum.

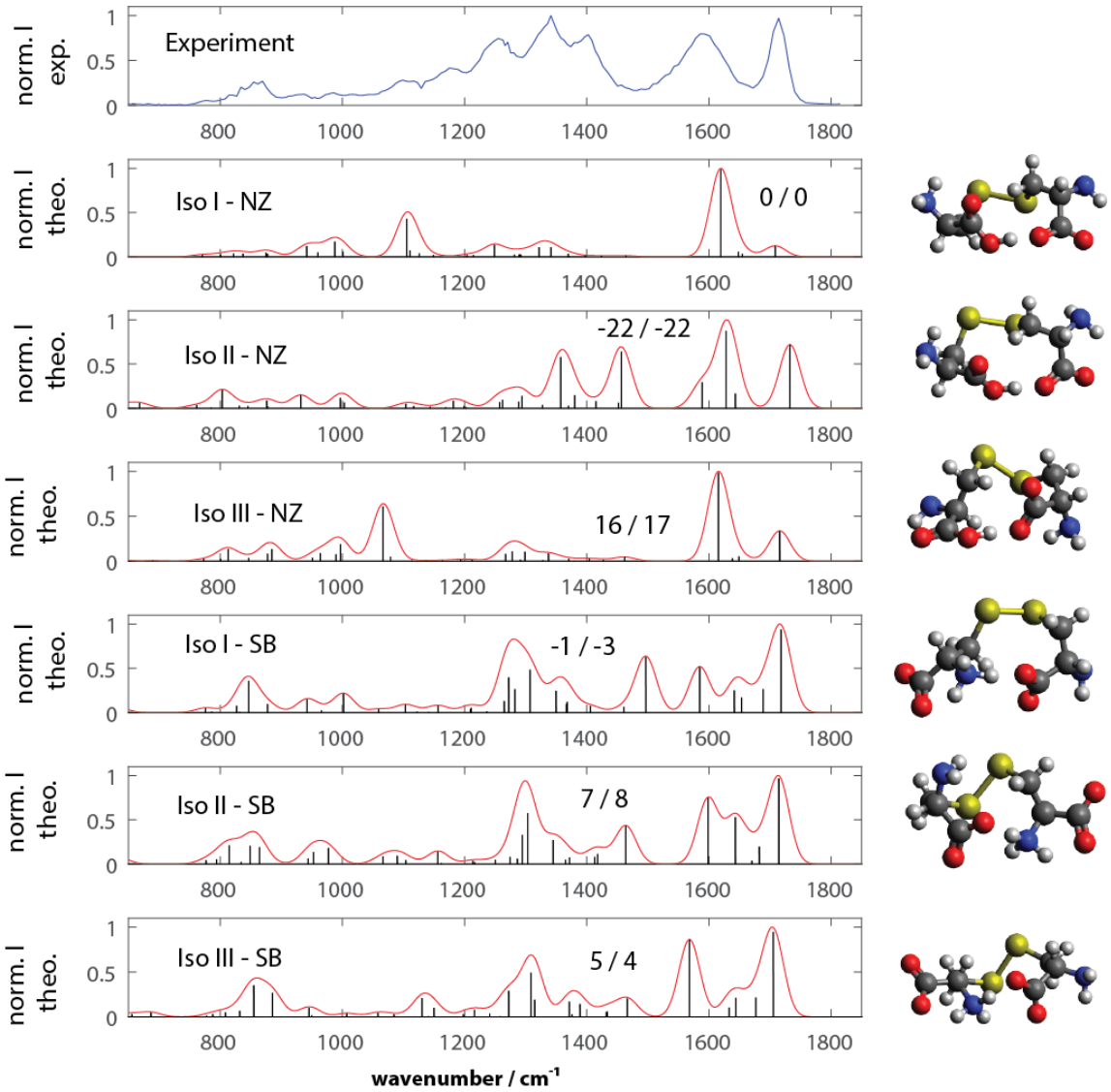

Figure S10. Comparison between experiment and theory for [2Cys-3H]$^-$ at the B3LYP/GCR level of theory. Harmonic frequencies were scaled with a uniform scaling factor of 0.987 and corresponding structures are shown to the right of every calculated spectrum.

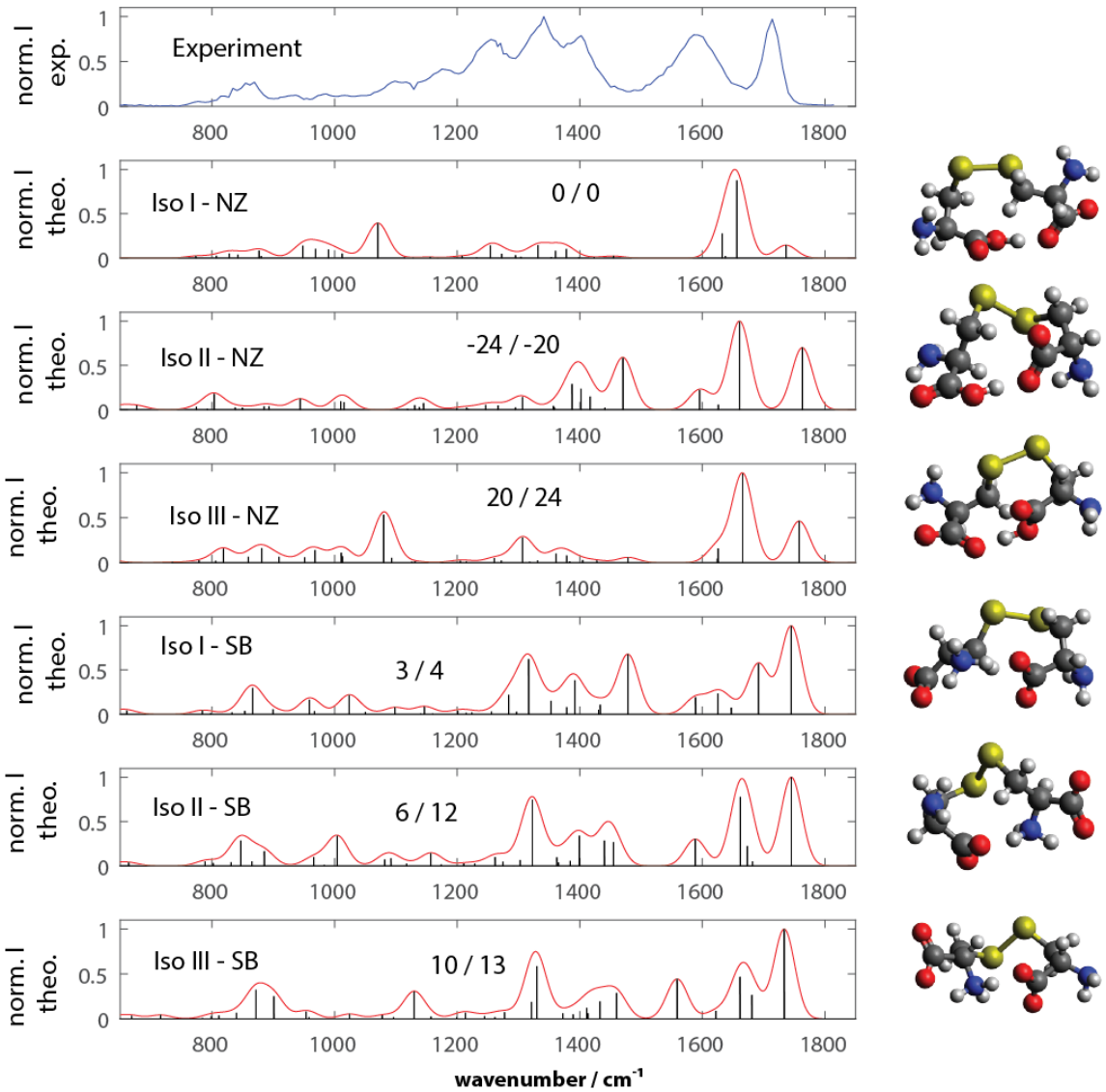

Figure S11. Comparison between experiment and theory for [2Cys-3H]$^-$ at the ωB97-D/GCR level of theory. Harmonic frequencies were scaled with a uniform scaling factor of 0.975 and corresponding structures are shown to the right of every calculated spectrum.

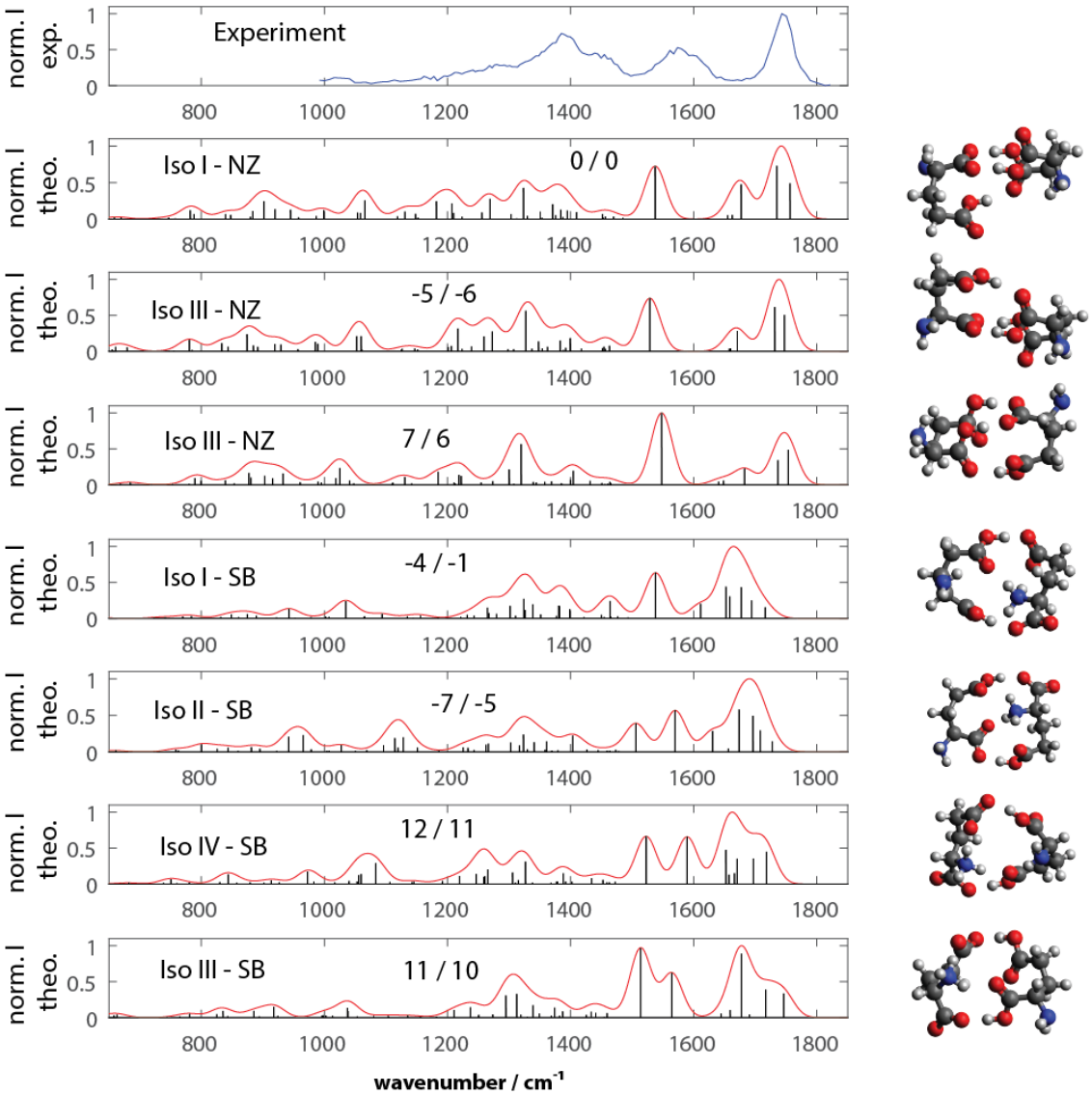

Figure S12. Comparison between experiment and theory for [2Glu-H]$^-$ at the B3LYP/GCR level of theory. Harmonic frequencies were scaled with a uniform scaling factor of 0.987 and corresponding structures are shown to the right of every calculated spectrum.

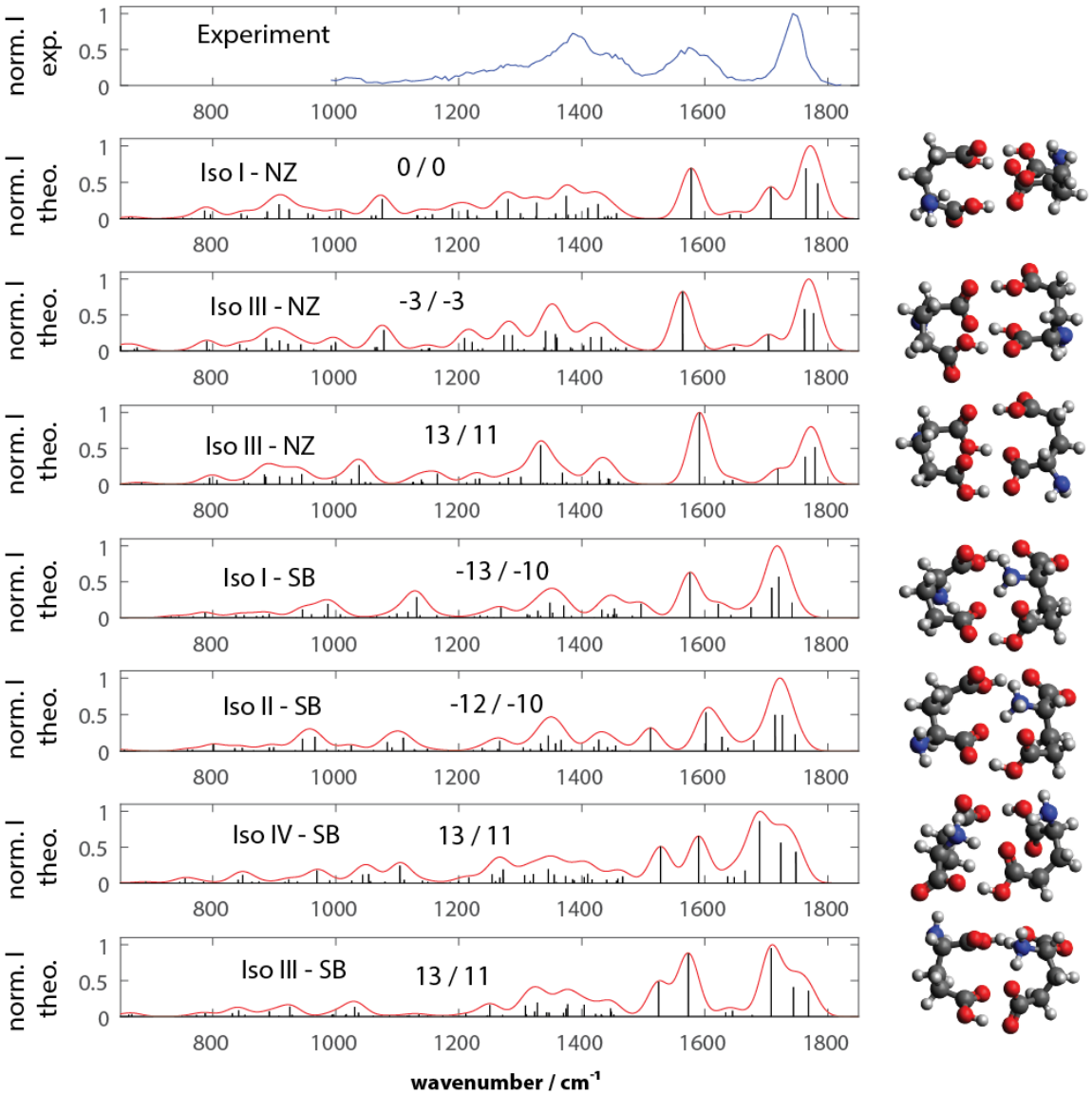

Figure S13. Comparison between experiment and theory for [2Glu-H]$^-$ at the ωB97-D/GCR level of theory. Harmonic frequencies were scaled with a uniform scaling factor of 0.975 and corresponding structures are shown to the right of every calculated spectrum.

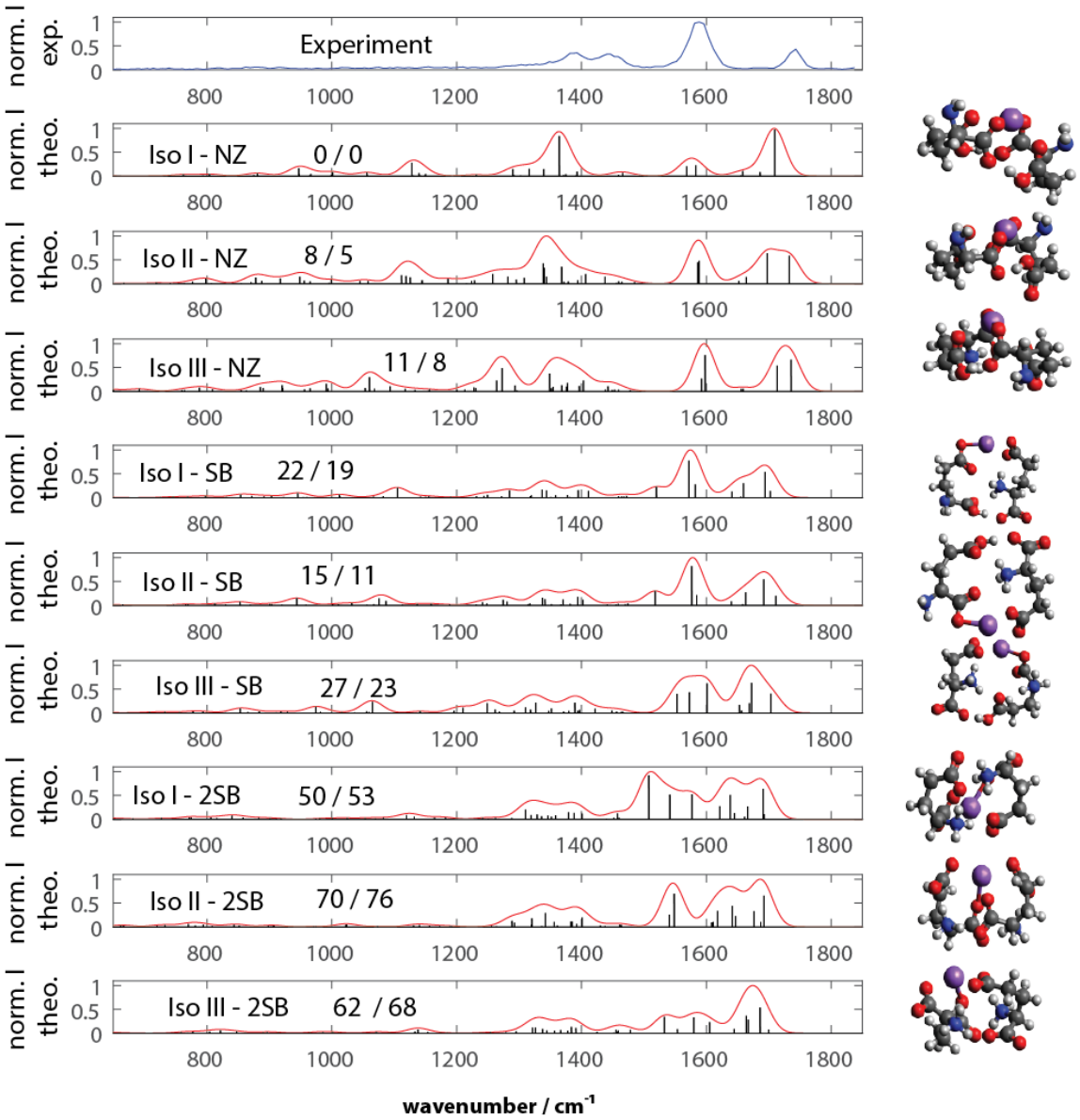

Figure S14. Comparison between experiment and theory for [2Glu-2H+Na]$^-$ at the B3LP/GCR level of theory (in kJ/mol). Harmonic frequencies were scaled with a uniform scaling factor of 0.987 and corresponding structures are shown to the right of every calculated spectrum. The label "2SB" donates isomers with two incorporated salt bridges.

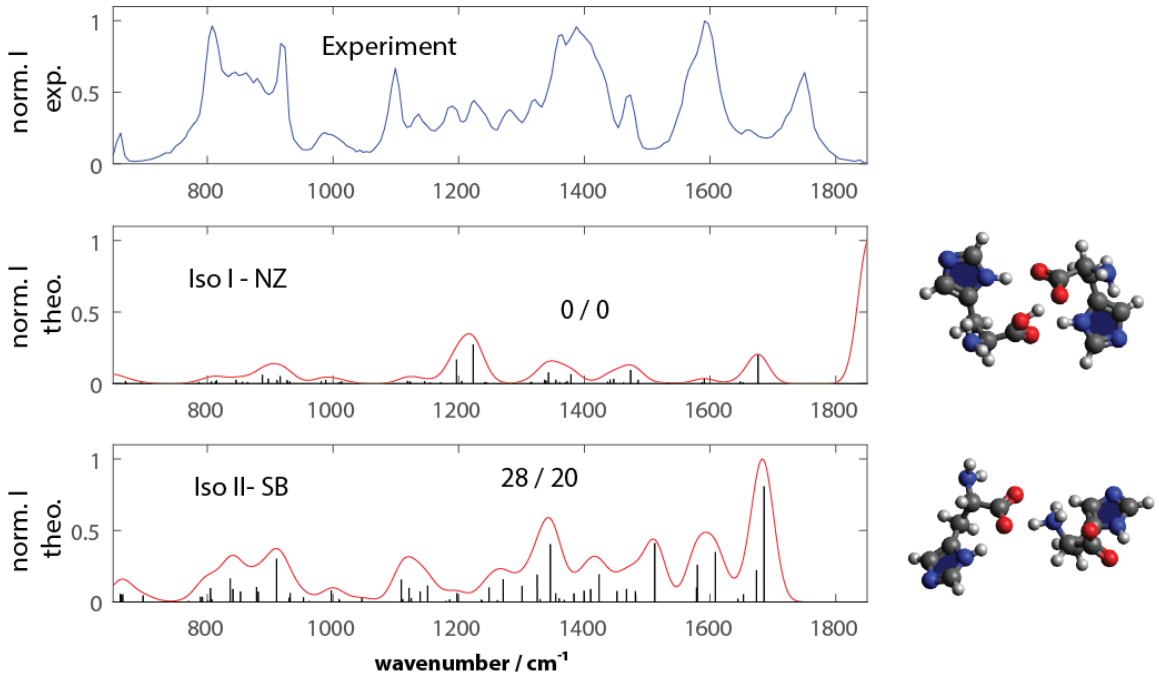

Figure S15. Comparison between experiment and theory for [2His-H]$^-$ at the B3LP/GCR level of theory (in kJ/mol). Harmonic frequencies were scaled with a uniform scaling factor of 0.987 and corresponding structures are shown to the right of every calculated spectrum.

Table S2. Comparison of the most intense experimental IRMPD transitions with predicted harmonic vibrations from B3LYP/6-311++G** calculations for [2Pro-H]$^-$ and peak assignments. Harmonic calculated frequencies were scaled with a uniform scaling factor of 0.987.

Experiment / cm^{-1}	Vibration (SBII)	Wavenumber / cm^{-1}	Vibration (NZII)	Wavenumber / cm^{-1}
1691	ν(SB)	1688	ν(C=O)	1784
1604	ν_{asym}(-COO$^-$), δ(-NH$_3^+$)	1625, 1603	ν_{asym}(-COO$^-$)	1689
			δ(C-O-H)	1512
1360	ν_{sym}(-COO$^-$)	1377	ν_{sym}(COO$^-$)	1386
1317	"Free" ν_{sym}(-COO$^-$)	1321	Ring bending modes	1365, 1356
1290-1210	NH$_3^+$, NH$_2$, CH$_2$ wagging	1146	O···H–O stretch combined with NH$_2$ + CH$_2$ wagging	1179, 1118, 1109

1210-1080	NH_2, CH_2 wagging	962	NH_2 + CH_2 wagging and rocking	975, 904

Table S3. Comparison of the most intense experimental IRMPD transitions with predicted harmonic vibrations from B3LYP/6-311++G** calculations for [2Phe-H]$^-$ and peak assignments. Harmonic calculated frequencies were scaled with a uniform scaling factor of 0.987.

Experiment / cm^{-1}	Vibration (SBII)	Wavenumber / cm^{-1}	Vibration (NZIII)	Wavenumber / cm^{-1}
1714	ν(SB)	1691	ν(C=O) coupled with ν(O-H)	1860
1602	ν_{asym}(-COO^-)	1583	ν(C=O) coupled with ν(O-H)	1693
1489	δ(-NH_3^+), ring bending modes	1502, ~1500	ν_{asym}(-COO^-), ring bending modes	1538, ~1500
1440-1390	ν_{sym}(-COO^-)	1379	ν_{sym}(-COO^-)	1424
1390-1270	"Free" ν_{sym}(-COO^-)	1316	δ(C-O-H)	1350
1270-1190	CH_2 wagging	1294	ν(C-OH), CH_2 wagging	1231
1190-1060	NH_3^+ + CH_2 wagging	1150	ν(C-OH), CH_2 wagging	1221

Table S4. Comparison of the most intense experimental IRMPD transitions with predicted harmonic vibrations from B3LYP/6-311++G** calculations for [2Cys-H]$^-$ and peak assignments. Harmonic calculated frequencies were scaled with a uniform scaling factor of 0.987.

Experiment / cm^{-1}	Vibration (SBIII)	Wavenumber / cm^{-1}	Vibration (NZI)	Wavenumber / cm^{-1}
1714	ν(SB)	1709	ν(C=O)	1784
1594	ν_{asym}(-COO^-)	1585	ν_{asym}(-COO^-)	1686
1450-1380	δ(-NH_3^+), NH_2 + CH_2 wagging	1484, 1394	δ(C-O-H)	1513

1380-1150	ν_{sym}(-COO$^-$), "Free" ν_{sym}(-COO$^-$)	1356, 1310	ν_{sym}(COO$^-$)	1384
890-810	Molecule breathing mode	861	NH_2 + CH_2 wagging and rocking	1160 - 1120

Table S5. Comparison of the most intense experimental IRMPD transitions with predicted harmonic vibrations from B3LYP/6-311++G** calculations for [2Cys-3H]$^-$ and peak assignments. Harmonic calculated frequencies were scaled with a uniform scaling factor of 0.987.

Experiment / cm^{-1}	Vibration (SBI)	Wavenumber / cm^{-1}	Vibration (NZII)	Wavenumber / cm^{-1}
1714	ν(SB)	1717	ν(C=O)	1732
1594	ν_{asym}(-COO$^-$)	1585	ν_{asym}(-COO$^-$)	1628
1402	δ(-NH_3^+)	1496	δ(C-O-H)	1456
1341	ν_{sym}(-COO$^-$)	1349	ν_{sym}(COO$^-$)	1357
1255	"Free" ν_{sym}(-COO$^-$)	1307		
1182	NH_3^+ + CH_2 wagging	1272	NH_2 + CH_2 wagging	1294
1100	NH_3^+ + CH_2 wagging and rocking	1001	Molecule breathing mode	932
890-810	C – C stretch	846	CH_2 rocking	803

Table S6. Comparison of the most intense experimental IRMPD transitions with predicted harmonic vibrations from B3LYP/6-311++G** calculations for [2Glu-H]$^-$ and peak assignments. Harmonic calculated frequencies were scaled with a uniform scaling factor of 0.987.

Experiment / cm^{-1}	Vibration (SBII)	Wavenumber / cm^{-1}	Vibration (NZII)	Wavenumber / cm^{-1}
1743	ν(C=O), ν(C=O), ν(SB)	1727, 1708, 1696	ν(C=O), ν(C=O), ν(C=O)	1747, 1731, 1671
1586	ν_{asym}(-COO$^-$)	1570	ν_{asym}(-COO$^-$)	1529
1490-1420	δ(-NH_3^+)	1506	ν_{sym}(COO$^-$)	1400
1420-1300	ν_{sym}(-COO$^-$), CH_2 wagging,	1403, 1361 1324	NH_2 + CH_2 wagging and rocking	1272

Free" ν_{sym}(-COO$^-$)			

xyz coordinates in Å at the B3LYP/GCR level of theory (Figure 3)

Structure: Atomic number x coordinate y coordinate z coordinate

[2Cys-H]$^-$ - NZ

7	3.230637625	-1.128024744	1.251354261
6	3.360325673	0.174722134	0.581980124
6	1.999173169	0.871366133	0.266244056
8	0.997465574	0.067457475	0.254003519
6	4.122925568	0.022194522	-0.737446198
16	5.851659505	-0.678563825	-0.496095508
8	2.004544233	2.082011372	0.038805397
1	3.097647386	-0.977344865	2.246183126
1	3.929369531	0.852181610	1.223229359
1	3.585033778	-0.640595402	-1.416472776
1	4.253162198	0.993354192	-1.210534211
1	5.421610865	-1.606566672	0.395562439
7	-3.812737481	1.623176714	-0.943961874
6	-3.624459658	0.861238356	0.294973227
6	-2.244844659	0.164731980	0.444262647
8	-2.141019823	-0.909907663	1.024636979
6	-4.783465240	-0.097154376	0.535230269
16	-4.948303170	-1.453008353	-0.763669722
8	-1.282959013	0.874926690	-0.064938326
1	-3.922056418	0.962811058	-1.710920908
1	-3.655238415	1.584799221	1.124243945
1	-4.682111567	-0.589866231	1.498066764
1	-5.729633407	0.440323442	0.485848591
1	-3.799927895	-2.081627114	-0.420548333
1	2.353501824	-1.533759204	0.925982669
1	-2.949828267	2.127380061	-1.129443232
1	-0.238752468	0.505381274	0.087833279

[2Cys-H]$^-$ - SB

7	3.615535961	-0.568655713	1.599038459
6	3.032376708	0.614013986	0.960591121
6	1.487132029	0.551893566	0.769965982
8	0.849979278	-0.223559094	1.527378380

6	3.769831650	0.977508401	-0.322178772
16	3.630529925	-0.316369213	-1.687176748
8	0.990004042	1.322229929	-0.102535702
1	2.928972021	-0.910108150	2.268314942
1	3.188312336	1.467165322	1.639419582
1	3.393402300	1.912165335	-0.726938816
1	4.841275068	1.052411584	-0.135908381
1	2.303500486	-0.144623059	-1.887335012
7	-1.602427108	0.928334594	0.509449528
6	-2.549499711	0.155137918	-0.357626234
6	-3.951584871	0.900215220	-0.261385860
8	-4.879501956	0.365544982	-0.878909564
6	-2.666637895	-1.297968901	0.054259250
16	-1.156059491	-2.372192179	-0.278537593
8	-3.916525158	1.951387217	0.433156144
1	-1.281167713	0.401385370	1.326426144
1	-2.198383610	0.225536664	-1.388234943
1	-2.925412054	-1.384510856	1.111666939
1	-3.466950396	-1.747176290	-0.528671512
1	-0.278855494	-1.683061826	0.505433372
1	3.687797690	-1.301025932	0.894833569
1	-0.683583511	1.208269277	0.064005261
1	-2.209504190	1.737637692	0.792780136

[2Cys-3H]$^{-}$ - NZ

7	3.009878794	-1.083387108	-0.744844388
6	1.980853162	-0.128412070	-0.329537275
6	2.613769865	1.273415094	-0.145340503
8	3.817186781	1.430775196	-0.261121411
6	1.314376037	-0.583397920	0.973078248
16	0.365236824	-2.201285541	0.825935126
8	1.799051584	2.266043971	0.127928336
1	3.821787268	-0.572580373	-1.076591977
1	1.189865866	-0.005480711	-1.079328465
1	2.085998217	-0.856481374	1.697927627
1	0.643454772	0.153336181	1.408976771
7	-3.033019130	0.867100623	-1.346237689
6	-2.711668256	0.620913037	0.064769991
6	-1.440552441	1.331059801	0.610313617
8	-1.295376459	1.356600969	1.841514258
6	-2.619561003	-0.882442469	0.334681317
16	-1.297967121	-1.782222924	-0.674676641
8	-0.635710440	1.771044132	-0.275831831
1	-2.166758845	0.752322883	-1.869686587
1	-3.552260216	0.974833559	0.673698034

1	-2.401474268	-1.079425572	1.382182767
1	-3.548889878	-1.372707884	0.040500139
1	2.667430164	-1.705897404	-1.464531312
1	-3.256460651	1.852791122	-1.451907512
1	0.780036205	2.054122325	0.042669297

[2Cys-3H]$^-$ - SB

7	-3.541173925	-0.832877777	1.311310488
6	-2.812642421	-0.999916738	0.051769926
6	-1.367149463	-1.559974178	0.190625176
8	-0.925744633	-1.801515262	1.320592587
6	-2.826870490	0.298594006	-0.751101193
16	-2.019830953	1.782449759	0.100413471
8	-0.749893491	-1.700625884	-0.921619311
1	-3.386089476	-1.669800804	1.867647308
1	-3.360677737	-1.726741349	-0.564134861
1	-2.320318596	0.172341928	-1.704505182
1	-3.853074919	0.637001391	-0.908632988
7	1.773378667	-1.145694045	-1.020389629
6	2.251667495	0.119787339	-0.369673271
6	3.503921087	-0.279263095	0.542131549
8	3.811224464	-1.495407136	0.454003705
6	1.164767497	0.830359774	0.414134550
16	0.077373589	1.825618979	-0.782665135
8	4.014906507	0.652174323	1.170994381
1	2.429789838	-1.841218574	-0.585266022
1	2.651849948	0.781250300	-1.142435896
1	0.529226327	0.136904255	0.962231488
1	1.633440075	1.537255574	1.092319669
1	-3.070482039	-0.101224802	1.841564957
1	0.712196960	-1.413797357	-0.874566642
1	1.932567514	-1.133535855	-2.023729422

[2Glu-H]$^-$ - NZ

7	-3.746011428	-1.301796544	1.490929858
6	-3.038381887	-1.531322009	0.222154937
6	-1.510492439	-1.291538542	0.283692556
8	-0.805320752	-1.938888318	-0.522688738
6	-3.674655752	-0.698595450	-0.918316910
6	-3.922974293	0.790565500	-0.616797457
6	-2.698875295	1.660895459	-0.371741821
8	-2.654968153	2.521638215	0.481290995
8	-1.117688729	-0.439123552	1.138648107
1	-3.487564261	-2.036781661	2.143267879

1	-3.165989245	-2.581809961	-0.051979635
1	-3.050386511	-0.798596169	-1.809124738
1	-4.648769950	-1.147377887	-1.141403407
1	-4.445455543	1.229842307	-1.476284839
1	-4.579755317	0.908452958	0.246103674
1	-3.372131722	-0.448524255	1.903094039
8	-1.711847309	1.399092100	-1.231528109
1	-0.844012714	1.756264649	-0.906801669
7	3.820244582	1.268889900	1.449245177
6	3.079776948	1.515235299	0.206986943
6	1.554102939	1.320237498	0.292074456
8	0.821519401	1.933523108	-0.481405926
6	3.664365537	0.679539917	-0.960352759
6	3.874427143	-0.819745667	-0.688905743
6	2.629061409	-1.664957857	-0.428217724
8	2.626751154	-2.584954393	0.365448262
8	1.604310295	-1.298599974	-1.183080499
8	1.179519293	0.477450854	1.211221470
1	0.173256975	0.112312104	1.141275665
1	3.532374761	1.946246634	2.149302816
1	3.218548385	2.565276466	-0.064242926
1	3.020708600	0.810570658	-1.832729003
1	4.642478010	1.110739119	-1.198067023
1	4.362626074	-1.257154011	-1.568943010
1	4.554370084	-0.977544891	0.150039131
1	3.542708453	0.365030437	1.823727803
1	0.707106305	-1.669189636	-0.867968026

[2Glu-H]$^-$ - SB

7	-1.217599993	-0.263229483	0.920683312
6	-2.596630305	-0.343672480	0.336729400
6	-2.832462929	-1.804668713	-0.204825715
8	-1.942377175	-2.645073378	0.125367184
6	-2.842863399	0.735237585	-0.721520189
6	-2.896171781	2.196109877	-0.206639009
6	-1.545495954	2.631727977	0.335754985
8	-1.257169179	2.516465849	1.522352697
8	-3.877672076	-1.973027140	-0.837348181
1	-0.952767848	-1.189146251	1.286742133
1	-3.296515110	-0.209964766	1.168372999
1	-2.080010960	0.656319615	-1.503120608
1	-3.798641048	0.482337748	-1.183382420
1	-3.175697694	2.845411837	-1.040178449
1	-3.644246675	2.290909985	0.584605086
1	-0.474379804	-0.024215062	0.205603606

8	-0.714007839	3.029288519	-0.601239896
7	4.302508462	1.494878992	-0.161978009
6	3.268832454	0.517057885	-0.539404690
6	1.821767590	1.070690701	-0.473645254
8	0.894394711	0.247359842	-0.677376606
6	3.484434215	-0.772182185	0.281822588
6	2.790572953	-2.047713508	-0.223469760
6	1.385952409	-2.268950705	0.307717875
8	1.045224129	-1.965245720	1.440148490
8	0.598094701	-2.887136086	-0.561816681
8	1.684525712	2.310395491	-0.261445052
1	3.427859814	0.266841183	-1.597391773
1	4.565315608	-0.943520102	0.281425433
1	3.189415009	-0.600838858	1.323089813
1	2.763840726	-2.087105072	-1.313653079
1	3.369128060	-2.919105620	0.110584227
1	3.994475825	2.404219096	-0.498878166
1	-0.355109808	-2.895056177	-0.246255078
1	-1.147509850	0.459073817	1.641678868
1	4.292859580	1.592469775	0.851522271
1	0.284712649	2.822852281	-0.364474819

[2His-H]$^-$ - NZ

7	-3.378422027	-2.028145563	1.463187305
6	-2.385299408	-2.083634168	0.389707459
6	-1.012281408	-1.435533759	0.695691233
8	-0.911191356	-0.781580046	1.784794668
6	-2.963870392	-1.489516239	-0.918369596
6	-3.452796321	-0.075561564	-0.825540613
7	-2.652265473	1.025271119	-0.589390380
6	-4.721176371	0.443934170	-0.970610723
6	-3.458190690	2.121240694	-0.599065573
7	-4.718941460	1.814134963	-0.831357618
8	-0.115408152	-1.591981599	-0.158749751
1	-2.893876386	-2.095524856	2.353619288
1	-2.162020362	-3.135872684	0.176898886
1	-2.192397828	-1.580509003	-1.687796536
1	-3.813383404	-2.106903181	-1.223884722
1	-1.649394929	1.055274731	-0.382644572
1	-5.630863914	-0.103312809	-1.171645864
1	-3.070382141	3.113968879	-0.427590342
7	3.447108208	2.048705953	1.399392874
6	2.415645067	2.100314230	0.367452231
6	1.049286668	1.481790225	0.713551924

8	0.086015195	1.719966322	-0.014192925
6	2.935891876	1.455344124	-0.946616347
6	3.409748274	0.038139780	-0.832125144
7	2.597608007	-1.057904813	-0.614516128
6	4.681641913	-0.483658514	-0.939748662
6	3.402011727	-2.153056885	-0.597776691
7	4.671559237	-1.851820007	-0.795239196
8	1.038646032	0.711489899	1.762190373
1	3.036082874	2.258242381	2.303631418
1	2.204483836	3.149965040	0.136018123
1	2.142346646	1.540288383	-1.694469808
1	3.781526493	2.055750686	-1.292185569
1	1.579756516	-1.093574041	-0.435047387
1	5.597512716	0.061168424	-1.119071007
1	3.007299898	-3.144475994	-0.434376120
1	-3.805278238	-1.104456717	1.465857091
1	3.799281865	1.097138207	1.469842499
1	0.157503948	0.066117604	1.801971535

[2His-H]$^-$ - SB

7	3.084405625	-3.002199658	1.158154807
6	3.024030177	-1.560765097	0.877256976
6	1.567402626	-1.010420184	0.869461770
8	1.431407830	0.266898498	0.927788976
6	3.735942415	-1.269272195	-0.475630395
6	4.354016181	0.090052341	-0.609814664
7	3.720818892	1.246291591	-0.216163793
6	5.565672098	0.507224750	-1.116026572
6	4.557463968	2.284976469	-0.488491208
7	5.683633256	1.878687414	-1.040329771
8	0.629273221	-1.820257803	0.795814686
1	2.297193945	-3.435666679	0.677257219
1	3.576531824	-1.040316771	1.665025863
1	4.527771445	-2.013760973	-0.579895992
1	3.026168356	-1.449705959	-1.294410100
1	2.809639159	1.221677853	0.261077717
1	6.354308492	-0.104450716	-1.529132800
1	4.301720751	3.309564073	-0.262915929
7	-1.236613631	0.481755036	1.078702183
6	-1.908916581	1.308099037	0.027116288
6	-3.113141030	2.051135791	0.726928248
8	-3.030374944	2.096482765	1.974119804
6	-2.279789780	0.482491576	-1.215470288
6	-3.378277262	-0.514471528	-1.008616148
7	-4.672700090	-0.127344612	-0.730397756

6	-3.425510924	-1.889676137	-1.062558314
6	-5.420765233	-1.257573508	-0.619582003
7	-4.704194076	-2.344929514	-0.821621494
8	-3.991924553	2.502614869	-0.038549231
1	-1.484645566	-0.508484252	1.011266836
1	-1.190233186	2.077448035	-0.268239189
1	-2.573270195	1.197275119	-1.989095553
1	-1.393419551	-0.043960548	-1.581285663
1	-4.915247902	0.847298861	-0.541857957
1	-2.610652993	-2.569304724	-1.262767828
1	-6.475273969	-1.233532359	-0.388768542
1	2.882411288	-3.147150790	2.143443964
1	-1.618216720	0.880318037	1.960061972
1	-0.168979073	0.500851866	1.038829068

[2Phe-H]$^-$ - NZ

7	-4.695331928	-1.645928137	-0.942763786
6	-3.395253343	-1.243259784	-1.483513635
6	-2.191066848	-1.759336192	-0.657246977
8	-2.352418505	-2.506906460	0.295211024
6	-3.340356744	0.283450759	-1.727082614
6	-3.527015894	1.138289364	-0.488256941
6	-2.476438057	1.340590966	0.419655961
6	-4.762344495	1.744828560	-0.224114860
6	-2.667231715	2.124892946	1.555844203
6	-4.952580549	2.531379981	0.912547657
6	-3.901935567	2.723330160	1.808001211
8	-1.048567283	-1.340751932	-1.134469095
1	-4.590142878	-2.581188717	-0.556178953
1	-3.281519821	-1.713353297	-2.469590409
1	-4.123670906	0.529604702	-2.450910361
1	-2.375284589	0.506824822	-2.184285520
1	-1.501312257	0.891085827	0.258709968
1	-5.583000443	1.597512026	-0.920361362
1	-1.837130255	2.261960214	2.240114971
1	-5.918216341	2.992881885	1.095131840
1	-4.043471453	3.334404043	2.694041969
1	-4.905735460	-1.062233221	-0.135865650
7	2.430931670	-2.042762235	2.728674054
6	2.634294517	-0.937222134	1.766060171
6	1.343637507	-0.664602150	0.951061627
8	0.715447025	0.382324252	1.149650766
6	3.839790557	-1.298995461	0.875450339
6	4.295118841	-0.202546638	-0.061567121
6	5.410484727	0.585742831	0.246574431

6	3.612384093	0.058356417	-1.257458584
6	5.836663686	1.601651292	-0.608741573
6	4.033575681	1.073364654	-2.113393475
6	5.148369316	1.849017821	-1.795179651
8	1.025287658	-1.619357600	0.150982134
1	1.697007843	-1.774222971	3.379712809
1	2.859819949	-0.033481594	2.338337290
1	4.662359637	-1.579761379	1.540139184
1	3.563294917	-2.185951563	0.296677596
1	5.951537787	0.398126882	1.169870734
1	2.737412273	-0.533574950	-1.502204573
1	6.704967049	2.198781468	-0.347757566
1	3.485307178	1.261601140	-3.030862161
1	5.474722383	2.639615576	-2.463155316
1	2.052136583	-2.832672068	2.208219208
1	-0.166974530	-1.506580709	-0.509417917

[2Phe-H]$^-$ - SB

7	-3.452930894	-0.741163578	2.486711919
6	-2.549764540	-1.391304376	1.529332673
6	-1.283060758	-0.560717219	1.156605311
8	-1.003524665	0.400247674	1.941157178
6	-3.316835594	-1.909174010	0.294529459
6	-4.061924585	-0.850496132	-0.491916116
6	-3.391117145	-0.020424277	-1.402735450
6	-5.441899822	-0.674104833	-0.330465809
6	-4.082444146	0.950056316	-2.124592989
6	-6.136346504	0.298282072	-1.051009314
6	-5.457298075	1.115010664	-1.952658036
8	-0.607616645	-0.924656864	0.169345790
1	-3.992537603	-0.032309812	1.994426303
1	-2.142039509	-2.283783302	2.024595238
1	-2.588040406	-2.398483754	-0.354004605
1	-4.032097094	-2.664959410	0.634839830
1	-2.320838897	-0.140936937	-1.528697799
1	-5.975878771	-1.309177100	0.369895314
1	-3.545073155	1.581857229	-2.824517677
1	-7.205703380	0.415897493	-0.906985494
1	-5.992034735	1.873092072	-2.515588320
1	-2.864207669	-0.212185056	3.126824596
7	1.349040352	1.274861218	1.057354879
6	2.510449712	0.882882326	1.918116685
6	3.553543356	2.067816498	1.865649447
8	3.103397107	3.117280030	1.335956164
6	3.077660218	-0.500109740	1.562917822

6	3.528522368	-0.654782650	0.124229534
6	2.693168648	-1.264885420	-0.821385175
6	4.784716608	-0.187363156	-0.288663814
6	3.109576158	-1.416943698	-2.145366534
6	5.199691742	-0.344976186	-1.608890085
6	4.365994551	-0.964286102	-2.541816856
8	4.659636265	1.830957184	2.376292692
1	1.384568877	0.814755428	0.146428528
1	2.134483335	0.844854123	2.943977538
1	3.925901202	-0.651768137	2.233603158
1	2.326689503	-1.263926515	1.786930000
1	1.706121564	-1.606278916	-0.522390520
1	5.419192745	0.314279555	0.434010535
1	2.447734897	-1.889593105	-2.863838424
1	6.175378039	0.021565742	-1.911551893
1	4.692058247	-1.086122623	-3.569857831
1	0.390453814	1.014660637	1.467668424
1	1.518677046	2.295918692	0.927442577

[2Pro-H]$^-$ - NZ

6	5.208577483	-0.618775204	0.421374506
7	4.437025581	0.623212238	0.237327891
6	3.275920661	0.324035384	-0.626992605
6	1.947312303	0.630168180	0.097737243
8	0.923551172	0.514511133	-0.693111064
6	3.382884113	-1.182057330	-1.003589642
6	4.238246951	-1.774076987	0.125968161
8	1.935578096	0.935731401	1.284467790
1	6.045293476	-0.645713829	-0.291330803
1	5.638610805	-0.653727069	1.426843880
1	3.289510836	0.937064425	-1.533280818
1	2.399490445	-1.641541981	-1.105733504
1	3.903573943	-1.289419677	-1.961744030
1	4.742923557	-2.702267707	-0.160330640
1	3.616814954	-1.979815648	1.003184532
6	-4.624272320	0.897135073	-0.863657175
7	-4.030198000	1.192149091	0.446277478
6	-3.485395298	-0.094705756	0.923932037
6	-2.022638395	-0.378927489	0.461608497
8	-1.606438799	-1.539956869	0.487928236
6	-4.495534222	-1.156645393	0.420304810
6	-5.389266481	-0.407315654	-0.601244495
8	-1.367604323	0.676867797	0.130880647
1	-5.272090932	1.716572432	-1.192410139
1	-3.861579177	0.733145228	-1.643983869

1	-3.440860214	-0.082371606	2.018815095
1	-3.948533869	-1.987528334	-0.026593044
1	-5.092228799	-1.563485904	1.240674889
1	-6.365885376	-0.179154492	-0.162690952
1	-5.560216112	-0.981099928	-1.516774197
1	4.042758788	0.918196160	1.128834085
1	-3.244638069	1.830977632	0.346491131
1	-0.090242643	0.565704926	-0.235673163

[2Pro-H]$^-$ - SB

6	4.926809539	-0.333526830	0.692251014
7	3.978312184	0.786188886	0.814697937
6	2.975802165	0.690713824	-0.271545510
6	1.529040778	0.537893090	0.253809196
8	0.626406660	0.630837164	-0.636306035
6	3.408182850	-0.518932705	-1.138123012
6	4.896538390	-0.682315468	-0.800528127
8	1.359742401	0.326951724	1.472908080
1	5.926063973	-0.042629139	1.036819280
1	4.616465227	-1.213887751	1.279536773
1	2.997221356	1.602031171	-0.879544154
1	2.858426129	-1.414613063	-0.829699216
1	3.207947463	-0.359744241	-2.198843202
1	5.499032430	0.038090428	-1.365269583
1	5.283758130	-1.684133437	-1.009527787
6	-1.818697699	-0.411531971	1.502903363
7	-1.870030665	0.405177823	0.250713779
6	-2.752750454	-0.305247240	-0.744427652
6	-4.064654512	0.541422122	-0.922290600
8	-4.076494508	1.620399383	-0.270028763
6	-2.991995231	-1.713052436	-0.154653626
6	-1.967738804	-1.843755638	0.987412392
8	-4.919329556	0.038946664	-1.667485725
1	-0.872380161	-0.211739438	2.007119675
1	-2.664465773	-0.124798688	2.133210141
1	-2.221276070	-0.344552647	-1.695652483
1	-4.015163191	-1.779828055	0.224019569
1	-2.879419844	-2.490467227	-0.911680787
1	-1.001943054	-2.190276706	0.607143781
1	-2.286498727	-2.532583861	1.774259804
1	3.461236669	0.733197243	1.689072924
1	-2.382011681	1.302254518	0.383243638
1	-0.866916252	0.550604336	-0.114132808

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