

Supplementary material

On peptide bond formation from protonated glycine dimers in the gas phase: computational insight into the role of protonation

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This PDF file contains:

I Supplementary Figure S1

II Cartesian coordinates of the stationary points

obtained for the mixed dimer $\text{H}^+\text{Gly}_2(\text{Gly})$

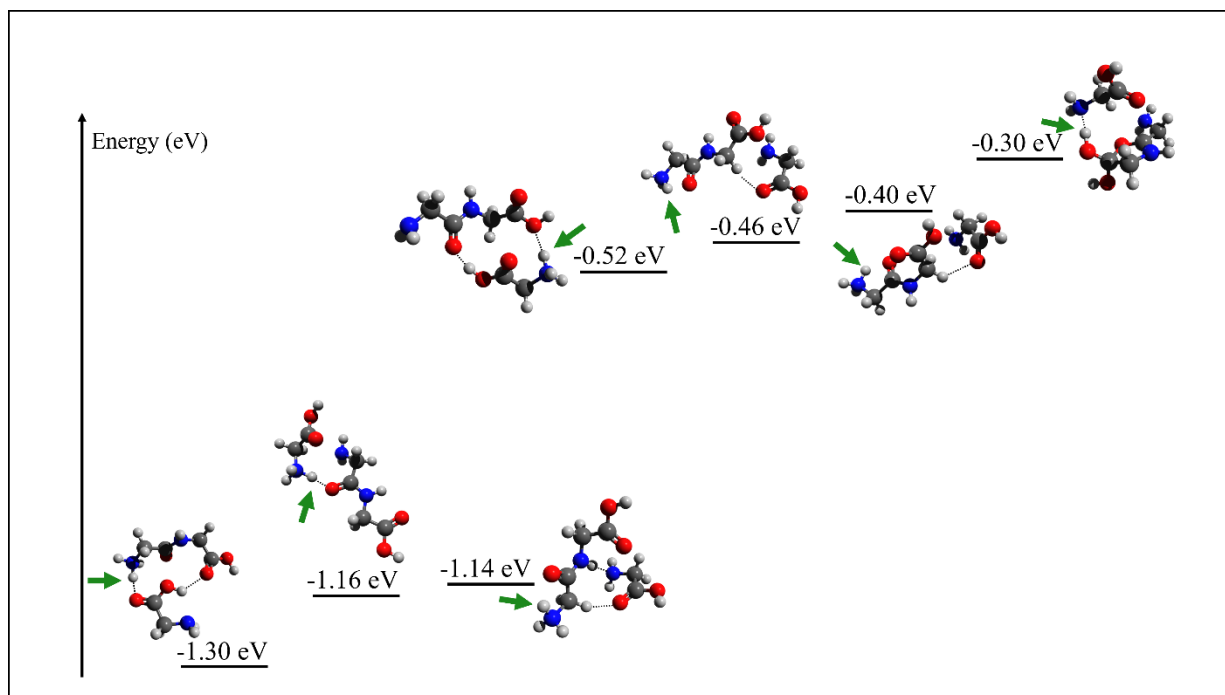


Figure S1. Conformers of the protonated cluster of dipeptide of glycine and glycine follow captions of main article: calculated at the DFT/M06-2X/6-311G++(2df,p) level of theory. The energies account for the harmonic zero-point correction scaled by the factor 0.9663. The green arrows point at the specific protonation site.

Table S1: Cartesian coordinates for the M06-2X structures of H⁺Gly₂(Gly) pathways in Å

Ground state

H	1.088269	-2.606336	-1.208998
H	3.087523	2.159815	-1.173959
O	1.018241	0.416756	0.412570
H	0.456446	1.228478	0.451727
O	-0.674058	-1.745699	-1.239032
O	-3.541817	1.630367	-0.472220
H	2.211799	-1.780995	-0.270398
O	-1.410721	1.573919	0.246343
C	2.260936	0.612257	0.002974
O	2.981120	-0.354057	-0.220470
N	1.558094	-2.611950	-0.297159
H	-3.429555	2.585049	-0.601243
C	-2.448243	1.007143	-0.005950
H	2.082046	-3.467355	-0.168490
H	-2.936858	-0.871648	-0.845590
C	2.714788	2.049983	-0.163717
C	-0.671126	-1.727672	-0.015404
H	3.555106	2.206345	0.501045
C	-2.743352	-0.468187	0.137491
H	1.234569	3.447548	-0.654450
C	0.464106	-2.425912	0.731767
N	-1.630063	-1.179435	0.740185
N	1.597256	2.940778	0.129510
H	0.837773	-1.817462	1.534519
H	-3.635671	-0.584114	0.734401
H	0.141278	-3.392453	1.088470
H	-1.528654	-1.135700	1.731726
H	1.714151	3.527121	0.932986

TS₁ – TS₂ pathway

Initial

C	1.403773	0.726009	0.028615
H	0.639303	0.941625	2.053476
O	1.173645	1.406837	-0.955720
C	0.306680	0.563736	1.088551
O	-2.722573	-0.529076	0.287373
H	0.016867	-0.481488	1.193720
C	-3.882791	-0.271983	0.025139
H	-1.132097	2.091690	1.229696
N	-0.861006	1.339344	0.599788
H	-4.953917	-1.971947	0.685865
C	-4.934307	-1.343645	-0.206259
H	-1.691145	0.693324	0.443781
N	-6.216646	-0.718622	-0.491822
H	-4.576531	-1.972344	-1.023526

H	-6.575483	-0.955537	-1.407350
H	-6.926276	-0.943516	0.192986
O	-4.308511	0.960221	-0.076313
H	-5.272574	0.889290	-0.294537
H	-0.553345	1.750234	-0.304035
C	4.801041	-0.628364	-0.065425
C	3.663854	0.174573	-0.651893
N	2.550016	0.097345	0.267743
O	4.728479	-1.209583	0.980557
H	3.984891	1.208062	-0.801684
H	3.400253	-0.228637	-1.632565
H	2.701544	-0.460367	1.100900
H	6.574910	-1.124461	-0.446816
O	5.867404	-0.601445	-0.852427

TS₁

C	0.421616	0.786634	0.039869
H	-0.008667	2.397132	-1.250916
O	-0.322592	-0.184237	0.251360
C	-0.068393	2.206270	-0.175550
O	-2.594479	-0.135788	1.640472
H	0.639037	2.886152	0.310983
C	-2.256718	-0.685155	0.724973
H	-1.730346	3.345315	0.059516
N	-1.447671	2.388887	0.253248
H	-1.632000	-2.526190	0.002347
C	-2.331821	-1.758020	-0.337047
H	-1.532234	2.269079	1.258932
N	-3.650432	-2.235428	-0.492467
H	-1.939949	-1.295050	-1.238662
H	-4.294108	-1.533202	-0.832194
H	-4.026173	-2.768656	0.278520
O	-3.351709	0.733373	-1.092260
H	-4.039524	1.170266	-1.600802
H	-2.774671	1.430383	-0.721020
C	3.861834	-0.465322	-0.088740
C	2.372195	-0.670095	0.075482
N	1.733862	0.621104	-0.040921
O	4.362270	0.606677	-0.275254
H	2.014658	-1.363072	-0.689557
H	2.176073	-1.124612	1.049384
H	2.357384	1.405137	-0.205229
H	5.465664	-1.448897	-0.105811
O	4.516793	-1.613973	0.002129

Intermediate 1

C	0.386984	0.487770	-0.058226
H	0.199428	2.562715	-0.467338
O	-0.165299	-0.684554	-0.048918
C	-0.450017	1.747912	-0.137280
O	-1.935584	-0.292134	1.310722

H	-0.757461	1.977819	0.886622
C	-1.581701	-0.804714	0.314739
H	-1.507224	1.947091	-1.893539
N	-1.588085	1.509389	-0.986682
H	-1.813455	-2.666450	-0.637994
C	-2.300206	-1.685837	-0.669502
H	-2.476152	1.741495	-0.550994
N	-3.707138	-1.800317	-0.450817
H	-2.087998	-1.266478	-1.656677
H	-4.164111	-0.895200	-0.430944
H	-3.937072	-2.311886	0.390989
O	-4.149676	1.290435	0.503883
H	-3.965848	0.909526	1.368959
H	-4.957428	1.803990	0.598112
C	3.975571	-0.105647	0.054518
C	2.552533	-0.630067	0.065755
N	1.679367	0.528720	-0.045870
O	4.229804	1.059811	-0.050491
H	2.399614	-1.314156	-0.771144
H	2.358204	-1.174687	0.991473
H	2.167449	1.422275	-0.121220
H	5.748330	-0.732131	0.161215
O	4.846471	-1.089178	0.171808

TS₂

C	0.347345	0.230902	-0.298399
O	-0.196516	-0.828088	0.100421
O	-2.139130	-0.104031	1.371717
C	-1.904516	-0.649597	0.366207
H	-2.136909	-2.717121	0.318162
C	-2.484578	-1.880271	-0.294910
N	-3.914362	-1.878814	-0.357342
H	-2.046639	-1.999475	-1.284410
H	-4.304680	-1.172642	-0.966805
H	-4.357701	-1.835958	0.550901
O	-3.033902	2.524325	0.724433
H	-3.108287	2.000845	1.529964
H	-3.525959	3.336310	0.874479
C	3.960430	-0.060223	0.085249
C	2.562214	-0.626368	0.217265
N	1.645911	0.376825	-0.293964
O	4.181244	1.022629	-0.377215
H	2.485703	-1.556038	-0.350475
H	2.349239	-0.854509	1.263510
H	2.083416	1.227679	-0.641252
H	5.749768	-0.523906	0.442746
O	4.865404	-0.909889	0.538439
H	-0.673881	2.075773	0.014721
H	-2.601589	1.373249	-0.788771
C	-0.554648	1.342199	-0.786443
N	-1.848399	0.732378	-1.048700

H	-0.119046	1.842676	-1.652427
H	-1.949762	0.410982	-2.006483

Intermediate 2

C	0.388801	-0.020053	-0.270454
O	-0.000855	-1.163485	-0.089165
O	-2.176563	0.282040	1.685602
C	-2.306183	-0.306199	0.672743
H	-3.937352	-1.617038	0.627046
C	-2.861174	-1.691497	0.443687
N	-2.612162	-2.147304	-0.909670
H	-2.441680	-2.315122	1.237380
H	-1.729554	-2.643039	-0.969664
H	-3.351014	-2.748960	-1.249109
O	-3.856867	2.353967	-0.144776
H	-3.951652	2.583781	0.785305
H	-4.474254	2.910339	-0.629266
C	4.025413	0.201960	0.062417
C	2.728210	-0.573496	0.049926
N	1.661798	0.359557	-0.240081
O	4.090693	1.379968	-0.148729
H	2.784664	-1.363547	-0.702593
H	2.580351	-1.055360	1.019086
H	1.947097	1.321934	-0.386271
H	5.869008	-0.058622	0.332800
O	5.056016	-0.586001	0.332718
H	-0.661568	1.798543	0.276851
H	-2.702782	1.150339	-0.720739
C	-0.636509	1.078353	-0.541749
N	-1.962581	0.426026	-0.617833
H	-0.440434	1.601433	-1.477389
H	-2.030975	-0.298965	-1.354969

Final (Gly₃)

C	-0.034584	-0.207457	-0.291224
O	0.535214	0.849062	-0.060793
O	2.445221	-1.016084	1.603918
C	2.680758	-0.389252	0.641265
H	4.492990	0.665800	0.643232
C	3.438282	0.907893	0.481017
N	3.242311	1.471334	-0.840726
H	3.121756	1.539342	1.314824
H	2.459609	2.116270	-0.848759
H	4.067786	1.950478	-1.176532
C	-3.657391	0.118007	0.080332
C	-2.254672	0.681234	0.110415
N	-1.347537	-0.389273	-0.245040
O	-3.900822	-1.023164	-0.193702
H	-2.180020	1.514906	-0.591298
H	-2.037612	1.071074	1.107556
H	-1.782467	-1.286038	-0.437123

H	-5.439658	0.649086	0.365765
O	-4.553928	1.041504	0.391320
H	0.736777	-2.197384	0.115985
H	2.835528	-1.733588	-0.977321
C	0.806535	-1.430119	-0.656284
N	2.213056	-0.963159	-0.720344
H	0.522048	-1.851172	-1.620345
H	2.369409	-0.163470	-1.372290

TS₃ pathway

Initial

H	4.325763	-1.350896	-0.119596
O	4.249228	-0.390272	-0.029775
C	2.971275	-0.041978	-0.025618
H	3.300032	1.895710	-0.767719
O	2.066207	-0.840581	-0.104403
C	2.802523	1.450790	0.097246
O	-2.674114	2.776383	0.007200
H	3.374994	1.766880	0.977267
C	-1.873155	1.739897	0.231958
N	1.398644	1.815226	0.101952
H	-0.973756	1.721286	-1.705633
C	-1.526840	1.033332	-1.067441
N	-0.723062	-0.134734	-0.809013
H	-2.450461	0.756045	-1.575643
H	0.277843	0.003185	-0.667401
O	-1.467056	1.412347	1.311308
H	-2.887108	3.201698	0.850843
H	1.300742	2.812114	-0.052975
H	0.962100	1.613695	0.997663
H	-1.239393	-4.285734	-0.057889
N	-1.328270	-3.447312	0.514356
C	-0.373704	-2.363189	0.133289
H	-1.267211	-3.714060	1.495776
H	-2.263072	-2.965122	0.317782
H	0.208882	-2.047727	0.994836
H	0.308859	-2.700940	-0.641873
O	-2.504121	-1.439507	-0.284545
C	-1.295191	-1.233076	-0.351897

TS₃

H	4.352659	-2.363656	0.476357
O	4.329040	-1.400429	0.574837
C	3.288349	-0.921056	-0.092328
H	4.083720	1.029343	-0.486176
O	2.504344	-1.583007	-0.714306
C	3.213319	0.587524	0.000072
O	0.361701	2.452095	-0.036503

H	3.208879	0.884653	1.047576
C	0.721110	0.742760	0.180230
N	1.987540	1.048271	-0.639296
H	0.024802	-0.864169	-1.031921
C	-0.364819	0.089833	-0.665365
N	-1.473868	-0.131742	0.245244
H	-0.686834	0.711972	-1.498046
H	-1.204255	-0.159400	1.226079
O	0.857705	0.431321	1.353158
H	0.365075	2.851740	0.841437
H	1.913384	0.685823	-1.588757
H	1.531753	2.173188	-0.500131
H	-5.513190	-1.496312	0.264040
N	-5.053087	-0.592793	0.160004
C	-3.790420	-0.472181	0.942285
H	-5.729511	0.142985	0.359665
H	-4.660587	-0.483616	-0.838634
H	-3.841260	0.382528	1.613125
H	-3.613892	-1.378028	1.518152
O	-3.121481	-0.262644	-1.309723
C	-2.718424	-0.273865	-0.148916

Intermediate

H	-4.958908	-0.841292	1.539202
O	-4.611571	-1.036303	0.656397
C	-3.541108	-0.285575	0.435599
H	-3.703375	-0.145334	-1.681232
O	-3.092431	0.494988	1.233304
C	-2.981097	-0.521121	-0.955066
O	-1.422731	2.592996	0.256085
H	-2.877805	-1.594494	-1.111541
C	-0.600400	-0.452750	-0.637661
N	-1.708340	0.125662	-1.137092
H	0.512186	1.328196	-0.148047
C	0.662842	0.398162	-0.701174
N	1.720813	-0.404340	-0.116798
H	0.900910	0.650250	-1.736897
H	1.411548	-1.320460	0.204877
O	-0.562548	-1.580096	-0.181309
H	-2.000417	2.058558	0.822407
H	-1.693626	1.134027	-1.242568
H	-1.565202	3.511399	0.496454
H	5.663548	0.016970	1.453106
N	5.264221	-0.195182	0.539589
C	3.986368	-0.959305	0.609799
H	5.978504	-0.644758	-0.031858
H	4.913949	0.706474	0.064367
H	4.069918	-1.888359	0.050076
H	3.734487	-1.180192	1.644687
O	3.404753	1.082987	-0.419351
C	2.965670	0.002162	-0.032153

Final (Gly₃)

H	-4.908448	-1.705954	0.634629
O	-4.716834	-0.957310	0.051558
C	-3.536876	-0.440569	0.388855
H	-3.950761	1.521955	-0.368715
O	-2.838959	-0.845778	1.271644
C	-3.195568	0.747292	-0.496922
H	-3.219996	0.424070	-1.537641
C	-0.806992	0.521507	-0.469597
N	-1.889638	1.265881	-0.172097
H	0.411648	0.891606	1.272957
C	0.499910	0.957401	0.185630
N	1.517201	0.045325	-0.295805
H	0.746726	1.988131	-0.078153
H	1.161691	-0.664130	-0.935439
O	-0.827306	-0.434198	-1.217816
H	-1.819192	1.927909	0.585838
H	5.403428	-1.356379	0.765637
N	5.041546	-0.614835	0.166438
C	3.737973	-0.951992	-0.475529
H	5.767760	-0.352731	-0.499678
H	4.759632	0.231253	0.757602
H	3.820726	-0.873491	-1.557490
H	3.436277	-1.962086	-0.206857
O	3.244761	0.917766	0.881712
C	2.770461	0.101596	0.097692

TS₄ pathway**Initial**

C	-0.524946	-0.245358	-0.397218
H	-0.218336	-2.339951	-0.718426
O	-0.085593	0.898269	-0.582392
C	0.370770	-1.467527	-0.417598
O	4.291478	-0.950576	0.610734
H	0.695859	-1.626992	0.615226
C	3.340468	-0.032360	0.697139
N	1.546256	-1.220352	-1.241304
H	3.585952	0.547556	-1.351810
C	3.491350	1.018366	-0.377300
N	2.275236	1.855410	-0.345504
H	4.376746	1.623684	-0.175997
H	2.151460	2.254657	0.587922
O	2.478393	0.006852	1.528019
H	4.223238	-1.558805	1.362470
H	1.346878	1.285675	-0.527541
H	1.282729	-1.150183	-2.220059
H	2.181130	-2.009773	-1.174439
H	-2.807010	1.221726	-0.939722
H	-5.904443	0.528307	0.546843

O	-4.309989	-1.164025	0.328570
C	-4.120096	0.015699	0.244004
O	-5.050657	0.952063	0.372628
N	-1.809282	-0.453380	-0.148774
C	-2.763433	0.624811	-0.025994
H	-2.181318	-1.388950	-0.027622
H	-2.499468	1.299346	0.791797
H	2.327386	2.619494	-1.018240

TS₄

C	-0.391693	-0.212496	-0.348218
H	0.149867	-2.250258	-0.823553
O	0.030991	0.899866	-0.674823
C	0.540007	-1.414413	-0.241330
O	3.943817	-1.218499	-0.004384
H	0.608708	-1.716192	0.804633
C	2.682959	-0.191173	0.273798
N	1.872678	-1.072152	-0.709769
H	3.163015	1.175561	-1.418120
C	3.181139	1.131408	-0.331103
N	2.243146	2.150553	0.220398
H	4.184015	1.337938	0.035040
H	2.197505	1.986873	1.235646
O	2.283432	-0.153063	1.436877
H	4.232575	-1.570900	0.850009
H	1.290132	1.932693	-0.149858
H	1.838404	-0.672460	-1.644896
H	2.971309	-1.735117	-0.515527
H	-2.694910	1.070145	-1.127258
H	-5.838395	0.406855	0.271786
O	-4.156555	-1.213340	0.365140
C	-4.017638	-0.046506	0.133027
O	-4.995593	0.847768	0.086777
N	-1.670236	-0.442211	-0.084200
C	-2.676332	0.593510	-0.144576
H	-2.006319	-1.368681	0.157328
H	-2.492442	1.375814	0.595616
H	2.518044	3.110562	0.017872

Intermediate

C	0.319708	0.239432	0.152672
H	-0.277743	2.004631	1.262145
O	-0.193961	-0.348181	-0.800231
C	-0.526985	0.944389	1.229361
O	-3.373254	2.291234	-1.210367
H	-0.303337	0.505568	2.202196
C	-2.370127	-0.494372	0.902706
N	-1.923530	0.777930	0.913709
H	-3.717264	0.004258	-0.775380
C	-3.395442	-0.843212	-0.173951
N	-2.582270	-1.766435	-1.040062

H	-4.238657	-1.396907	0.232489
H	-2.328074	-2.587211	-0.479543
O	-1.893124	-1.404697	1.543187
H	-2.965056	2.666031	-1.996955
H	-1.682522	-1.282711	-1.261832
H	-2.321084	1.412469	0.227667
H	-4.068138	2.909630	-0.962500
H	2.433340	0.096459	-1.616328
H	5.762125	-0.273828	-0.602547
O	4.205132	0.672657	0.853416
C	3.967698	0.029705	-0.128979
O	4.880405	-0.494237	-0.937985
N	1.635272	0.318210	0.317352
C	2.568736	-0.287783	-0.602777
H	2.043791	0.804408	1.108052
H	2.440776	-1.372093	-0.645893
H	-3.067586	-2.061819	-1.886930

Final (Gly₃)

C	-0.042084	-0.335621	-0.318984
H	0.382160	-2.362331	-0.983038
O	0.495839	0.750046	-0.543682
C	0.768671	-1.644710	-0.260420
H	0.680097	-2.076601	0.736627
C	2.766414	-0.515001	0.318441
N	2.153955	-1.353605	-0.549159
H	3.886374	0.443337	-1.341236
C	3.733853	0.513652	-0.266740
N	3.005186	1.793808	0.028554
H	4.684296	0.517704	0.262148
H	2.922879	1.884580	1.047658
O	2.478100	-0.406985	1.486492
H	2.028652	1.692814	-0.330593
H	2.394707	-1.263886	-1.524855
H	-2.209479	1.193143	-1.089636
H	-5.418169	0.764749	0.253473
O	-3.902476	-1.012082	0.264275
C	-3.648285	0.146806	0.099801
O	-4.535317	1.132841	0.098050
N	-1.346576	-0.461269	-0.116741
C	-2.248518	0.667671	-0.132808
H	-1.773861	-1.364129	0.062157
H	-1.997998	1.389924	0.647788
H	3.462912	2.620807	-0.355885

TS_s pathway

Initial

H	-0.447368	-1.637309	-0.780293
O	0.537300	-2.000512	-0.847662
C	1.270904	-1.438731	0.045732

H	3.079017	-1.731856	-1.128038
O	0.928364	-0.668447	0.917548
C	2.751151	-1.777828	-0.091926
O	0.541021	2.645037	0.838359
H	2.970074	-2.762045	0.320691
C	0.823575	1.959308	-0.089100
H	4.470003	-0.904542	0.782212
N	3.466334	-0.735142	0.703851
H	0.170006	0.357900	-1.395118
C	-0.173981	1.318608	-1.025007
H	3.033199	-0.684911	1.634713
N	-1.452017	1.178932	-0.379213
H	-0.245282	1.983154	-1.894196
H	-1.829469	2.007263	0.061232
O	2.122670	1.761979	-0.479704
H	2.634713	2.468326	-0.054459
H	3.287342	0.185039	0.274411
C	-2.132548	0.031538	-0.236434
C	-3.488576	0.155823	0.451344
N	-4.174246	-1.076209	0.707886
O	-1.737002	-1.059758	-0.650304
H	-3.338095	0.698659	1.389502
H	-4.110756	0.798894	-0.179015
H	-4.345420	-1.593949	-0.145381
H	-3.650433	-1.676380	1.332522

TS₅

H	3.733314	-2.704298	-0.164203
O	4.099585	-1.813455	-0.273557
C	3.149170	-0.913455	-0.106265
H	3.950135	0.588806	-1.332705
O	2.001533	-1.199747	0.145637
C	3.674512	0.489589	-0.279639
O	0.168353	0.276363	1.728301
H	4.605413	0.565900	0.290859
C	0.072183	0.129990	0.632637
H	2.960021	2.381986	-0.303784
N	2.662413	1.482666	0.060543
H	-0.046780	-1.048548	-1.039189
C	-0.275045	-0.005944	-0.809326
H	2.615913	1.595015	1.069693
N	-1.643937	0.320142	-1.012912
H	0.411698	0.657463	-1.332985
H	-1.860487	1.254846	-1.329235
O	-0.400986	2.713894	0.048931
H	-0.938614	3.355352	0.524568
H	0.406356	3.180202	-0.187631
C	-2.564690	-0.412097	-0.279037
C	-4.029280	-0.088747	-0.518557
N	-4.960734	-0.808516	0.299530
O	-2.155821	-1.256390	0.484016

H	-4.163828	0.989769	-0.379427
H	-4.234010	-0.281412	-1.576091
H	-4.906017	-1.806724	0.137885
H	-4.799716	-0.649730	1.286625

Intermediate

H	5.069908	0.860300	0.133053
O	4.556400	0.051105	0.284776
C	3.312753	0.223547	-0.107503
H	2.400154	-1.230781	1.191284
O	2.849570	1.218753	-0.594904
C	2.470235	-1.013370	0.125475
O	0.487740	0.349262	1.543196
H	2.889476	-1.878493	-0.387745
C	0.451326	0.405255	0.367750
H	0.484716	-1.598657	-0.280284
N	1.112562	-0.729146	-0.392457
H	-0.055415	1.280358	-1.540245
C	-0.173997	1.500737	-0.476973
H	1.153635	-0.500554	-1.387481
N	-1.562793	1.643451	-0.125877
H	0.368321	2.418955	-0.252344
H	-1.933050	2.542453	0.139699
O	-0.484947	-2.811892	-0.244087
H	-0.511966	-3.651381	0.222590
H	-1.367905	-2.412256	-0.238456
C	-2.343757	0.540683	-0.154888
C	-3.821255	0.727185	0.153606
N	-4.612217	-0.467277	0.191032
O	-1.832141	-0.539911	-0.428247
H	-3.897890	1.251293	1.111057
H	-4.223241	1.412043	-0.599894
H	-4.590368	-0.971695	-0.685808
H	-4.334040	-1.093536	0.935016

Final (Gly₃)

H	-5.021670	0.692213	0.375591
O	-4.155845	1.046313	0.633891
C	-3.209658	0.509798	-0.105596
H	-1.660230	1.018219	1.315258
O	-3.352332	-0.301519	-0.976627
C	-1.841188	1.066867	0.243487
O	-1.094654	-1.367242	1.181629
H	-1.763832	2.100955	-0.092929
C	-0.510220	-1.056278	0.210294
H	0.126142	0.689808	-0.637568
N	-0.845930	0.246518	-0.476970
H	0.625128	-1.625102	-1.534686
C	0.654181	-1.777690	-0.451740
H	-1.252328	0.001109	-1.393219
N	1.918852	-1.312290	0.087575

H	0.541010	-2.837519	-0.235081
H	2.510800	-1.982775	0.555584
C	2.385595	-0.063263	-0.132795
C	3.823394	0.214697	0.281711
N	4.237248	1.582442	0.225798
O	1.678607	0.795764	-0.661104
H	3.970261	-0.181544	1.291253
H	4.457287	-0.391089	-0.375316
H	4.137564	1.977912	-0.700456
H	3.739859	2.169807	0.882270

TS₆ – TS₇ pathway

Initial

O	-2.928386	-0.336542	1.580644
O	-4.301523	1.046288	0.462488
O	0.100729	-0.831712	-0.415261
N	-2.299572	-1.756204	-0.498232
N	-1.503395	1.331312	-0.996191
C	-3.527580	-0.934712	-0.620086
C	-3.634900	0.062974	0.511954
C	-0.269925	1.549401	-0.258015
C	0.588248	0.297325	-0.273939
H	-2.183292	2.049593	-0.766278
H	-1.333909	1.402713	-1.994997
H	-3.091544	0.275881	2.313987
H	-2.293910	-2.257529	0.392539
H	-4.405500	-1.582824	-0.593797
H	-3.505457	-0.390952	-1.558835
H	-0.516331	1.739726	0.790652
H	0.323870	2.401018	-0.605627
H	-1.370110	-1.174151	-0.514839
H	2.295088	1.393976	-0.004599
N	1.889772	0.468485	-0.094050
H	2.804517	-1.236250	-0.922870
H	2.575726	-1.299595	0.821177
C	2.818949	-0.635105	-0.011030
C	4.202809	-0.061144	0.191434
O	4.426531	1.113689	0.259646
O	5.113581	-1.020791	0.281919
H	5.985757	-0.618801	0.411830
H	-2.245608	-2.447833	-1.246423

TS₆

O	2.318964	-0.181813	1.445248
O	3.847344	-1.243508	0.075160
O	0.012796	0.969281	-0.591902
N	2.307262	2.070067	0.139231
N	1.865163	-1.035199	-0.777010
C	3.315008	1.059977	-0.298977

C	2.909172	-0.333180	0.184693
C	0.523257	-1.372139	-0.322805
C	-0.406258	-0.167902	-0.354006
H	2.821473	-1.772730	-0.643294
H	1.847911	-0.607469	-1.701785
H	2.731521	-0.846590	2.013701
H	2.270729	2.076652	1.161824
H	4.276516	1.288447	0.157667
H	3.412501	1.101950	-1.382334
H	0.581266	-1.755983	0.695838
H	0.123190	-2.164252	-0.958634
H	1.352862	1.754278	-0.195094
H	-2.027030	-1.358248	0.042541
N	-1.686493	-0.416977	-0.127552
H	-2.728198	1.141841	-1.084846
H	-2.499647	1.366565	0.647210
C	-2.694859	0.619998	-0.125782
C	-4.030362	-0.038706	0.138946
O	-4.159081	-1.216827	0.313379
O	-5.011035	0.851939	0.151300
H	-5.850954	0.400454	0.324423
H	2.518683	3.008986	-0.197801

Intermediate 1

O	2.735587	-0.384331	1.370939
O	4.083839	-1.102485	-0.358963
O	-0.127990	1.144487	-0.219809
N	2.276065	1.957916	0.181952
N	1.780773	-0.945824	-0.643129
C	3.262710	1.051187	-0.454463
C	2.947400	-0.388635	-0.016313
C	0.521151	-1.182870	0.007304
C	-0.481963	-0.038553	-0.098474
H	3.834518	-2.023112	-0.507502
H	1.737011	-0.786590	-1.639514
H	3.520876	-0.753544	1.791395
H	2.394778	1.926754	1.196571
H	4.269390	1.318900	-0.137174
H	3.185892	1.147509	-1.536503
H	0.698134	-1.361768	1.068875
H	0.067468	-2.090745	-0.397112
H	1.251266	1.608011	-0.028272
H	-2.060198	-1.332868	0.036418
N	-1.761778	-0.365206	-0.029172
H	-2.792725	1.215414	-0.960804
H	-2.739949	1.308210	0.795832
C	-2.821945	0.618016	-0.046913
C	-4.138786	-0.120094	0.031704
O	-4.222807	-1.313662	0.091992
O	-5.163183	0.721251	0.024381
H	-5.989370	0.217466	0.075851

H	2.382509	2.921771	-0.131007
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Intermediate 2

O	2.961669	-0.815216	1.235675
O	3.827120	-0.429702	-0.882752
N	3.717957	1.688982	0.659839
C	2.436050	1.123850	0.103418
C	2.693524	-0.378848	-0.065347
H	3.948640	-1.328385	-1.214323
H	3.124755	-1.766985	1.234005
H	2.224092	1.602722	-0.847347
H	1.637580	1.323434	0.811011
H	3.933748	1.214955	1.543901
H	3.669586	2.697200	0.814307
H	4.480841	1.475947	0.007049
H	0.550212	-1.321621	1.090927
C	0.387983	-1.297216	0.010984
N	1.667732	-1.170944	-0.663672
H	-2.673126	1.555491	0.301066
C	-0.571682	-0.153675	-0.320002
N	-1.855060	-0.361889	-0.004373
O	-0.164908	0.878738	-0.829649
H	1.544109	-0.894485	-1.632838
H	-2.178451	-1.240087	0.382771
O	-4.345774	-1.029125	0.627052
C	-2.868354	0.634523	-0.253866
C	-4.201993	0.070179	0.171536
O	-5.182311	0.945105	-0.024299
H	-0.065720	-2.251510	-0.263882
H	-6.019151	0.545065	0.254525
H	-2.911058	0.903931	-1.312287

TS₇

O	3.125671	-0.189516	1.413756
O	3.730615	-1.197519	-0.588825
N	4.456963	1.389573	0.255326
C	3.317687	1.097435	-0.633893
C	2.814362	-0.284549	-0.211731
H	3.498582	-2.089978	-0.300502
H	2.354937	0.055473	1.942295
H	3.582256	1.063379	-1.689939
H	2.546304	1.848612	-0.474527
H	3.911502	0.656310	1.237455
H	4.614973	2.382105	0.394881
H	5.319614	0.964948	-0.077952
H	0.271419	1.020465	-1.052454
C	0.410049	0.320146	-0.225224
N	1.516314	-0.582737	-0.464600
H	-3.406028	-1.342685	-0.674784
C	-0.843007	-0.552507	-0.064928
N	-2.005920	0.104413	-0.059116

O	-0.734586	-1.755829	0.063660
H	1.223595	-1.556141	-0.374942
H	-2.066262	1.104942	-0.203225
O	-4.182739	1.604314	-0.145781
C	-3.262422	-0.589335	0.103601
C	-4.371065	0.432346	0.025752
O	-5.562242	-0.133146	0.171452
H	0.529345	0.902604	0.697292
H	-6.245684	0.551046	0.115181
H	-3.313426	-1.107473	1.064381

Intermediate 3

O	-2.588494	-1.085134	1.782689
O	-3.723858	1.376682	0.001134
N	-4.561382	-1.157309	-0.253977
C	-3.347521	-0.749135	-0.935535
C	-2.809302	0.518322	-0.346013
H	-3.384923	2.185050	0.413364
H	-2.448643	-1.290247	2.710666
H	-3.463458	-0.540734	-2.011152
H	-2.596511	-1.530247	-0.827358
H	-3.502002	-1.331282	1.572413
H	-4.879581	-2.050407	-0.612879
H	-5.312546	-0.488122	-0.383898
H	-0.391759	-0.474691	-1.507053
C	-0.455448	-0.150073	-0.467194
N	-1.552121	0.785870	-0.271534
H	3.420913	1.465729	-0.450175
C	0.804972	0.631183	-0.071906
N	1.955248	-0.025920	-0.187745
O	0.697016	1.779713	0.320466
H	-1.193670	1.682737	0.087804
H	2.003391	-0.986359	-0.508725
O	4.090612	-1.553782	-0.447065
C	3.217219	0.585906	0.164743
C	4.302945	-0.442075	-0.051483
O	5.497605	0.046427	0.249918
H	-0.595824	-1.010481	0.191751
H	6.167812	-0.636509	0.097516
H	3.224343	0.911065	1.207709

Final (Gly₃)

O	4.093835	-1.358942	-0.182639
N	3.247009	1.980993	0.471318
C	3.834469	0.975028	-0.383640
C	3.229937	-0.382939	-0.142621
H	3.711703	-2.245831	-0.097206
H	4.917674	0.851479	-0.300095
H	3.624757	1.208027	-1.433934
H	3.281542	2.896878	0.042438
H	3.722027	2.040146	1.364321

H	0.878225	0.943760	-0.866448
C	0.862227	0.343559	0.043481
N	1.977353	-0.597691	0.066613
H	-2.872247	-1.409547	-0.700841
C	-0.383200	-0.552180	0.102914
N	-1.554263	0.068255	0.017672
O	-0.243515	-1.757709	0.235381
H	1.598525	-1.550889	0.207713
H	-1.630536	1.073184	-0.095293
O	-3.739833	1.521361	-0.232843
C	-2.805110	-0.655228	0.086421
C	-3.924007	0.347065	-0.076114
O	-5.110146	-0.240828	-0.021012
H	0.906847	1.012972	0.900704
H	-5.802935	0.428310	-0.126922
H	-2.914902	-1.172283	1.042592

TS₈ – TS₉ pathway

Initial

O	-1.790468	1.491221	-0.988186
O	-0.294818	2.457151	0.373369
O	-2.064329	-1.695186	-0.548404
O	-4.150730	-0.891100	-0.585524
N	1.515628	0.589168	-0.005522
N	-1.445748	-0.316692	1.708879
C	0.317405	0.475144	-0.817696
C	-0.608612	1.584032	-0.385979
C	-2.840587	-0.376723	1.300161
C	-2.945482	-1.055284	-0.041756
H	-1.374370	0.081466	2.638172
H	-1.067506	-1.258133	1.746451
H	-2.325333	2.260736	-0.741940
H	1.489972	1.317580	0.701978
H	-0.174775	-0.488724	-0.681049
H	0.559646	0.597477	-1.876558
H	-3.254154	0.629138	1.215737
H	-3.499399	-0.930613	1.982044
H	-4.182369	-1.381084	-1.419801
O	2.702706	-1.018563	-1.072800
N	4.798581	-0.905597	0.193982
C	3.801839	0.079441	0.702092
C	2.581092	-0.151647	-0.211864
H	5.066411	-1.608050	0.882412
H	4.189684	1.091296	0.607014
H	3.568282	-0.124157	1.744761
H	4.227286	-1.357388	-0.599720
H	5.644577	-0.475662	-0.178272

TS₈

O	0.873350	0.459852	1.334311
O	0.323857	2.253056	0.002479
O	2.351362	-1.545075	-0.649303
O	4.147346	-1.447963	0.689652
N	-1.611557	0.506646	-0.353129
N	2.033027	1.121910	-0.676937
C	-0.281009	0.018806	-0.689858
C	0.674087	0.956032	0.054116
C	3.230729	0.592265	-0.038599
C	3.172725	-0.920253	-0.038920
H	1.559143	2.242491	-0.525378
H	1.970104	0.792162	-1.638559
H	0.909573	1.228500	1.917810
H	-1.647858	1.511287	-0.188781
H	-0.129538	0.086093	-1.769343
H	-0.168974	-1.015001	-0.373046
H	3.312780	0.959968	0.981698
H	4.117540	0.918289	-0.585265
H	4.089682	-2.413887	0.643570
O	-2.702100	-1.488041	-0.333031
N	-4.923243	-0.739218	0.347357
C	-3.974387	0.405563	0.256653
C	-2.656982	-0.268485	-0.181919
H	-5.702819	-0.677699	-0.305859
H	-3.870115	0.888736	1.225693
H	-4.322162	1.130123	-0.476264
H	-4.253355	-1.543271	0.066437
H	-5.293086	-0.891351	1.284537

Intermediate 1

O	-0.000964	1.107832	1.375766
O	0.224795	2.455257	-0.499448
O	2.766022	-0.899909	-1.327005
O	3.609554	-2.010068	0.424420
N	-1.431323	0.363126	-0.861357
N	2.030285	1.265476	0.269286
C	0.008309	0.156854	-0.759309
C	0.597445	1.260943	0.125098
C	2.650428	0.097284	0.859621
C	2.998476	-0.976522	-0.152523
H	0.727597	3.182247	-0.112723
H	2.460059	1.489491	-0.623354
H	0.427415	1.711616	1.994708
H	-1.724432	1.268637	-1.206234
H	0.464264	0.198224	-1.746522
H	0.178389	-0.823866	-0.321181
H	1.994662	-0.334724	1.618441
H	3.574107	0.375833	1.372356
H	3.842507	-2.656094	-0.258225
O	-2.084528	-1.484020	0.297979
N	-4.487679	-1.050484	0.448391

C	-3.780653	0.048489	-0.267143
C	-2.309534	-0.415144	-0.260845
H	-5.168333	-1.542800	-0.128701
H	-3.898818	0.986044	0.272294
H	-4.169982	0.155612	-1.277112
H	-3.648246	-1.691106	0.670198
H	-4.944031	-0.750093	1.308720

Intermediate 2

O	0.712138	1.739336	1.238776
O	0.517080	2.254456	-1.016625
N	-1.384469	0.670734	0.001640
C	-0.011119	0.138383	-0.258481
C	0.949018	1.320259	-0.074320
H	1.144542	2.986897	-1.067276
H	1.362644	2.406956	1.491414
H	0.025500	-0.252532	-1.271449
H	0.177647	-0.655875	0.461728
H	-1.386084	1.105356	0.934574
N	2.339599	1.062700	-0.272131
H	2.541804	0.927041	-1.257075
H	-1.549513	1.444741	-0.657002
H	2.675139	0.171869	1.598351
C	2.962234	0.042601	0.555886
H	4.046498	0.168453	0.506139
H	-4.816400	-1.645153	0.775774
N	-4.935711	-0.793389	0.243087
H	-5.151451	-1.024844	-0.717923
H	-3.711404	0.392306	1.432808
C	-3.850086	0.117557	0.379261
H	-4.066094	1.057483	-0.143809
O	-2.215719	-1.421892	-0.579479
C	-2.512386	-0.382748	-0.123873
C	2.677137	-1.401256	0.174149
O	2.713253	-2.317214	0.936113
H	2.312456	-2.473957	-1.338516
O	2.394497	-1.529414	-1.137742

TS₉

O	-0.121999	1.785936	1.162545
O	0.939572	2.529010	-0.722649
N	-1.439326	0.725021	-0.498848
C	-0.020766	0.390914	-0.766823
C	0.833853	1.403721	0.025278
H	1.364874	3.238784	-0.221611
H	0.113805	1.355407	1.998117
H	0.232814	0.459673	-1.821473
H	0.140452	-0.622731	-0.413267
H	-1.068505	1.404952	0.602674
N	2.049083	0.999031	0.599984
H	2.828350	1.403274	0.095575

H	-1.872733	1.303641	-1.214339
H	1.417793	-0.804884	1.489802
C	2.289570	-0.376180	0.986064
H	3.103377	-0.411738	1.711557
H	-4.665887	-1.186700	1.148569
N	-4.621137	-1.227731	0.138395
H	-4.370600	-2.169770	-0.134338
H	-4.081750	0.762599	-0.143163
C	-3.746420	-0.244861	-0.417087
H	-3.786145	-0.280528	-1.512969
O	-1.795461	-1.213975	0.645827
C	-2.285959	-0.363757	-0.028343
C	2.649039	-1.266049	-0.195341
O	2.558604	-0.914382	-1.337198
H	3.285371	-3.004242	-0.558787
O	3.059600	-2.459679	0.210780

Intermediate 3

O	-0.031707	2.519161	0.096904
O	0.350912	-2.040665	0.840953
N	1.341928	-0.586380	-1.181053
C	-0.067773	-0.510954	-0.910084
C	-0.371939	-1.029603	0.469433
H	0.175860	-2.371925	1.733390
H	0.766084	2.157096	0.506374
H	-0.622258	-1.139628	-1.609386
H	-0.437496	0.513664	-0.992021
H	0.067054	3.474632	0.074767
N	-1.311828	-0.547202	1.226274
H	-1.471953	-0.994871	2.121575
H	1.667250	-1.063721	-2.006774
H	-1.713470	1.403987	0.548643
C	-2.255947	0.505625	0.861342
H	-2.839478	0.760485	1.743760
H	4.491841	0.147757	1.192647
N	4.598026	0.508052	0.252429
H	4.463148	1.510519	0.289112
H	3.937940	-1.185943	-0.754086
C	3.693872	-0.121784	-0.665423
H	3.825325	0.303220	-1.664975
O	1.800079	0.491600	0.718043
C	2.217741	-0.027535	-0.306457
C	-3.172252	0.034632	-0.253992
O	-2.975047	-0.955379	-0.897538
H	-4.734797	0.587326	-1.152588
O	-4.173505	0.882011	-0.418723

Final (Gly₃)

O	-0.380285	2.093255	1.142661
N	-1.993451	0.962552	-0.842698
C	-0.660602	1.431070	-1.099847

C	0.153673	1.419705	0.168931
H	0.099379	2.049881	1.983499
H	-0.693269	2.467051	-1.444744
H	-0.157758	0.826363	-1.855709
N	1.317569	0.868496	0.269133
H	1.856157	0.926338	1.139400
H	-2.791577	1.512441	-1.118428
H	2.204990	0.391655	-1.599395
C	1.899631	-0.085689	-0.667354
H	1.180186	-0.882273	-0.871664
H	-3.273021	-1.950271	1.609816
N	-3.646171	-2.017971	0.671186
H	-3.156444	-2.767140	0.197670
H	-4.115425	-0.002118	0.474564
C	-3.538786	-0.777643	-0.039666
H	-3.987650	-0.880240	-1.032862
O	-1.118424	-0.841890	0.119067
C	-2.124546	-0.252700	-0.234488
C	3.122111	-0.660943	0.025780
O	3.450286	-0.326540	1.128571
H	4.507266	-1.899991	-0.280741
O	3.732505	-1.540579	-0.740910