Supporting information

Structure of the $[M + H - H_2O]^+$ Ion from Tetraglycine: a Revisit by means of Density Functional Theory and Isotope Labeling

Udo H. Verkerk,[a] Junfang Zhao,[a] Michael J. Van Stipdonk,[b] Benjamin J. Bythell,[c†] Jos Oomens,[d,e] Alan C. Hopkinson,[a] and K.W. Michael Siu[a]*

[a] Department of Chemistry and Centre for Research in Mass Spectrometry, York University, 4700 Keele Street, Toronto, Ontario, Canada M3J 1P3; [b] Department of Chemistry, Wichita State University, Wichita, Kansas 67260-0051, U.S.A.; [c] Computational Proteomics Group, German Cancer Research Center (DKFZ), Im Neuenheimer Feld 580, 69120, Heidelberg, Germany; [d] FOM Institute for Plasma Physics, 3430 BE Nieuwegein, The Netherlands; and [e] University of Amsterdam, Science Park 904, 1098XH Amsterdam, The Netherlands.

[†] Current Address: Ion Cyclotron Resonance Program, National High Magnetic Field Laboratory, Florida State University, 1800 East Paul Dirac Dr., Tallahassee, FL 32310-4005, U.S.A.

* To whom correspondence should be addressed. Tel: (416)650-8021; FAX: (416)736-5936; E-mail: kwmsiu@yorku.ca

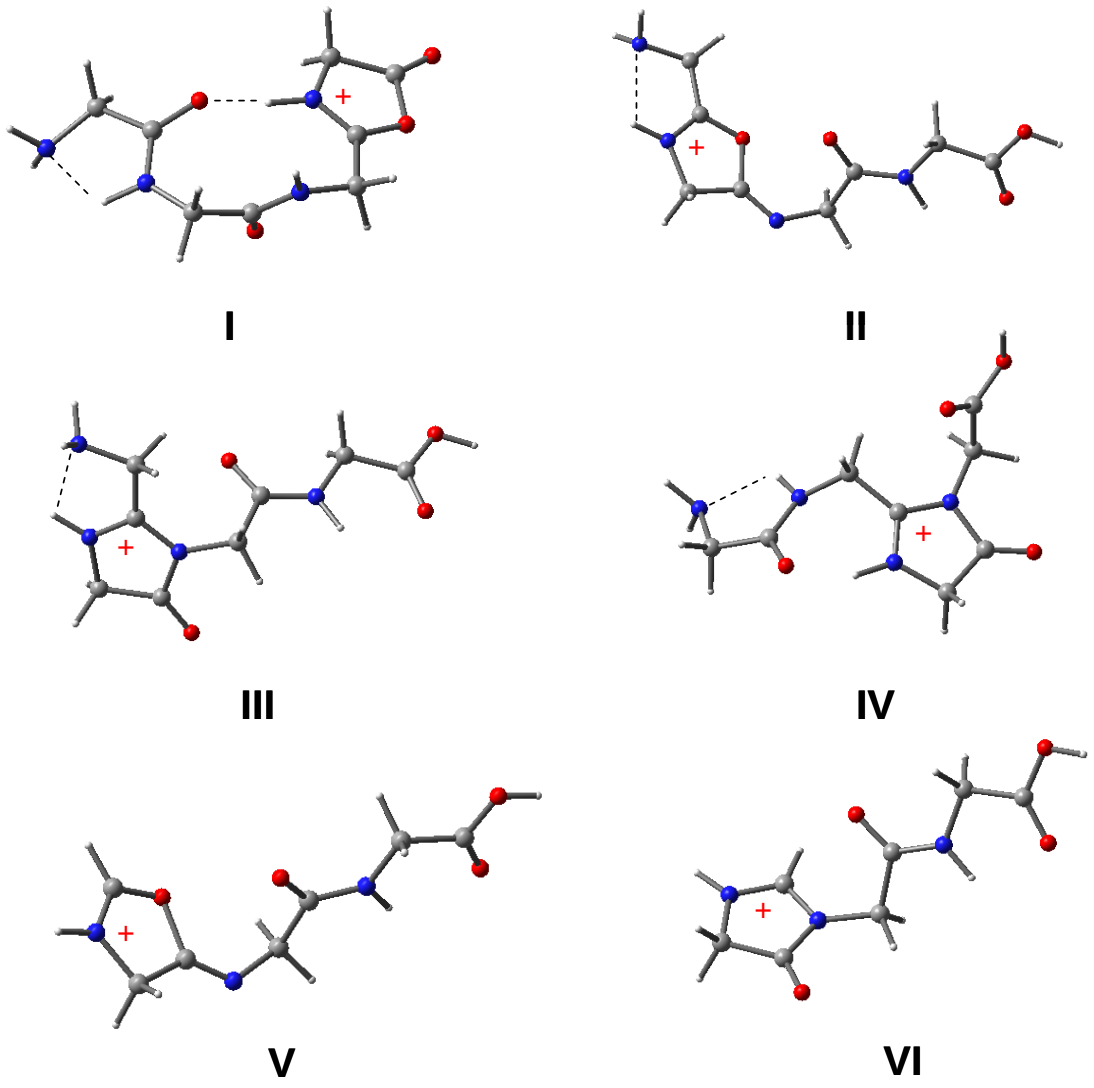

Figure S1: Optimized structures of $[GGGG + H - H_2O]^+$ (**I** – **IV**) and $[GGGG + H - H_2O - 29]^+$ (**V** – **VI**) determined at the B3LYP/6-311++G(d,p) level of theory.

Tables of total energies and Cartesian coordinates of the optimized structures of **I-VI** at the B3LYP/6-311++G(d,p) level of theory

I	E_t= -832.6402588		
7	-4.550769	-1.459923	0.498336
6	-3.262473	-1.859689	-0.062178
6	-2.340803	-0.671321	-0.325094
8	-1.199061	-0.845944	-0.792229
7	-2.850585	0.525860	-0.029950
6	-2.152272	1.778102	-0.245653
6	-0.729921	1.716774	0.317758
7	0.263027	2.106197	-0.551531
6	1.642428	1.969267	-0.165290
6	2.103487	0.540339	-0.139883
8	3.362120	0.296153	0.171972
7	1.395645	-0.516288	-0.390243
6	2.200217	-1.720085	-0.219845
1	-2.711381	-2.542107	0.591995
1	-3.373941	-2.378959	-1.018410
1	-2.143389	2.034270	-1.310042
1	-2.689042	2.566071	0.285538
1	2.293405	2.523900	-0.845517
1	1.807856	2.369099	0.840845
1	1.810370	-2.356386	0.578655
6	3.556834	-1.157655	0.157926
1	2.265085	-2.304631	-1.140637
8	4.594429	-1.636732	0.402413
8	-0.475267	1.336525	1.441406
1	0.042340	2.331912	-1.509609
1	0.353598	-0.535162	-0.575410
1	-5.332677	-1.762084	-0.068709
1	-4.691789	-1.808773	1.438104
1	-3.794410	0.497518	0.351972

II	E_t= -832.615714785		
7	-5.018075	1.918180	-0.018294
6	-3.753924	1.674100	-0.694700
6	-3.175344	0.373181	-0.224033
8	-2.045663	-0.083372	-0.675175
7	-3.745835	-0.383590	0.669422
6	-2.948557	-1.579536	0.947725
6	-1.737752	-1.335221	0.070603
7	-0.700116	-1.981216	-0.048679
6	0.447174	-1.521690	-0.801661
6	1.139798	-0.379821	-0.012639
8	0.495066	0.392319	0.679562
7	2.470363	-0.303418	-0.198067
6	3.280391	0.737393	0.406798

1	-5.799600	1.973039	-0.659454
1	-5.003813	2.763624	0.538478
1	-3.845353	1.615624	-1.784749
1	-2.999042	2.443251	-0.497012
1	-4.632016	-0.095836	1.078900
1	-2.663700	-1.633894	1.999539
1	-3.482785	-2.489571	0.665598
1	1.122387	-2.362552	-0.955590
1	0.162773	-1.117416	-1.779674
1	2.974647	1.731489	0.067450
1	2.975806	-0.993025	-0.742031
6	4.728193	0.500190	0.025771
1	3.186187	0.731726	1.496710
8	5.102345	-0.415156	-0.664011
8	5.528004	1.434638	0.552828
1	6.442255	1.244839	0.288337

III	E_t= -832.656246772		
7	3.652418	-2.491576	0.095900
6	2.425454	-1.840512	0.530891
1	1.538003	-2.247753	0.039086
1	2.254249	-1.915070	1.611043
6	2.475877	-0.380098	0.163682
7	3.484260	0.106904	-0.517112
1	4.237972	-0.521186	-0.789617
6	3.334008	1.533228	-0.772222
1	4.136091	2.119340	-0.317261
1	3.287786	1.757017	-1.840465
6	1.996589	1.829274	-0.099109
8	1.379340	2.845205	-0.032889
7	1.583748	0.580547	0.477971
6	0.265378	0.412117	1.077785
1	0.341613	-0.212882	1.970510
1	-0.067610	1.404904	1.382823
6	-0.699288	-0.246530	0.066328
8	-0.255409	-0.956250	-0.826877
7	-2.000224	-0.009240	0.283189
6	-3.049868	-0.592826	-0.535921
1	-2.925219	-0.325789	-1.589059
1	3.473209	-3.280071	-0.513007
1	4.225611	-2.808187	0.868147
1	-2.319212	0.629044	1.005034
1	-3.040183	-1.684925	-0.479144
6	-4.382856	-0.070513	-0.033840
8	-4.494757	0.697690	0.888830
8	-5.397344	-0.570814	-0.743641
1	-6.230122	-0.212376	-0.396660

IV	E_t= -832.653515593		
7	4.448536	-1.296438	-1.059573
6	4.356725	-0.170494	-0.129146
6	2.929986	0.081060	0.350139
8	2.669647	0.959620	1.174989
7	1.987994	-0.713875	-0.214623
6	0.634158	-0.849184	0.297166
6	-0.216287	0.383518	0.093935
7	0.178029	1.567831	0.486592
6	-0.821569	2.590220	0.206025
6	-1.940383	1.780100	-0.433326
8	-3.011591	2.118440	-0.827828
7	-1.440681	0.430908	-0.480324
6	-2.285191	-0.674782	-0.905481
1	4.959057	-0.311403	0.773137
1	4.704237	0.763239	-0.579801
1	2.370662	-1.412915	-0.851204
1	0.168878	-1.703666	-0.187979
1	0.632813	-1.049723	1.374788
1	-1.168393	3.079671	1.119402
1	-0.447176	3.351429	-0.483039
1	-3.169975	-0.238368	-1.372207
6	-2.690911	-1.545257	0.283211
1	-1.786256	-1.288013	-1.659906
8	-2.175580	-1.470341	1.368781
8	-3.653267	-2.394480	-0.068918
1	-3.890980	-2.951045	0.691237
1	1.118814	1.660807	0.922585
1	4.868271	-1.032029	-1.942194
1	4.990054	-2.063957	-0.680649

V	E_t= -737.8949923		
6	-3.639718	-1.110899	0.793908
8	-2.605698	-0.376314	0.982549
7	-4.367538	-0.804392	-0.244483
6	-3.801926	0.347330	-0.962518
6	-2.548471	0.619464	-0.161895
7	-1.648989	1.433591	-0.318708
6	-0.409125	1.432982	0.425040
6	0.428277	0.201576	-0.021607
8	-0.116043	-0.825240	-0.395654
7	1.757046	0.366961	0.084683
6	2.700978	-0.693658	-0.219192
1	-5.205241	-1.303893	-0.516543
1	-3.556696	0.085681	-1.993149
1	-4.490932	1.194807	-0.949267
1	0.117541	2.366174	0.230846
1	-0.580590	1.341215	1.503097
1	2.548303	-1.562600	0.427411
1	2.167493	1.251854	0.361134

6	4.103427	-0.154362	-0.015973
1	2.590452	-1.040545	-1.250653
8	4.345121	0.973225	0.335935
8	5.024169	-1.088187	-0.276664
1	5.904808	-0.704690	-0.137247
1	-3.859813	-1.923591	1.478017

VI	E_t= -737.94210810		
6	-2.512977	-1.098478	0.557899
7	-3.645260	-1.207017	-0.098651
1	-4.171233	-2.067001	-0.173021
6	-4.030095	0.069573	-0.702177
1	-4.097170	0.003791	-1.790385
1	-4.978428	0.436912	-0.302380
6	-2.876462	0.977696	-0.282768
8	-2.660634	2.115708	-0.549289
7	-2.032001	0.149398	0.538677
6	-0.695800	0.542195	0.968259
1	-0.577816	1.595888	0.712056
1	-0.604909	0.437801	2.052040
6	0.340789	-0.369653	0.269670
8	-0.016493	-1.450011	-0.187065
7	1.593710	0.093812	0.256040
6	2.709095	-0.662642	-0.292853
1	2.834617	-1.617636	0.224579
1	1.833560	1.011145	0.620465
1	2.553347	-0.887131	-1.351594
6	3.963934	0.175736	-0.129416
8	3.970527	1.272356	0.371941
8	5.035108	-0.458440	-0.609114
1	5.816252	0.105673	-0.489676
1	-2.042342	-1.916256	1.081998