Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information

Doubly Charged Protonated *a* Ions Derived from Small Peptides

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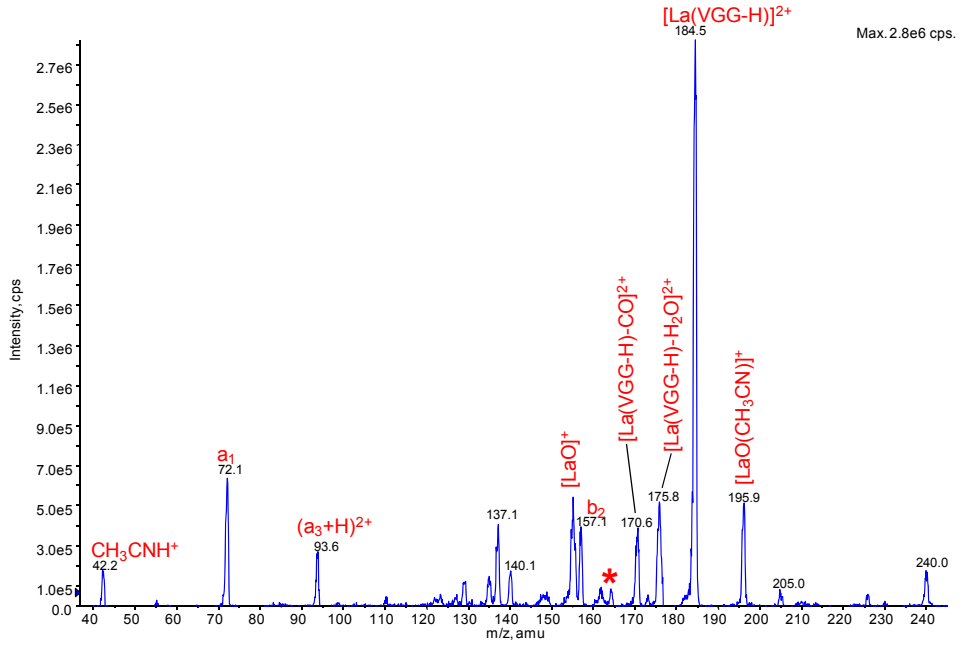

Figure S1a. CID of $[La(VGG)(CH_3CN)_3]^{3+}$ (*m/z* 164.2) at collision energy 51 eV.

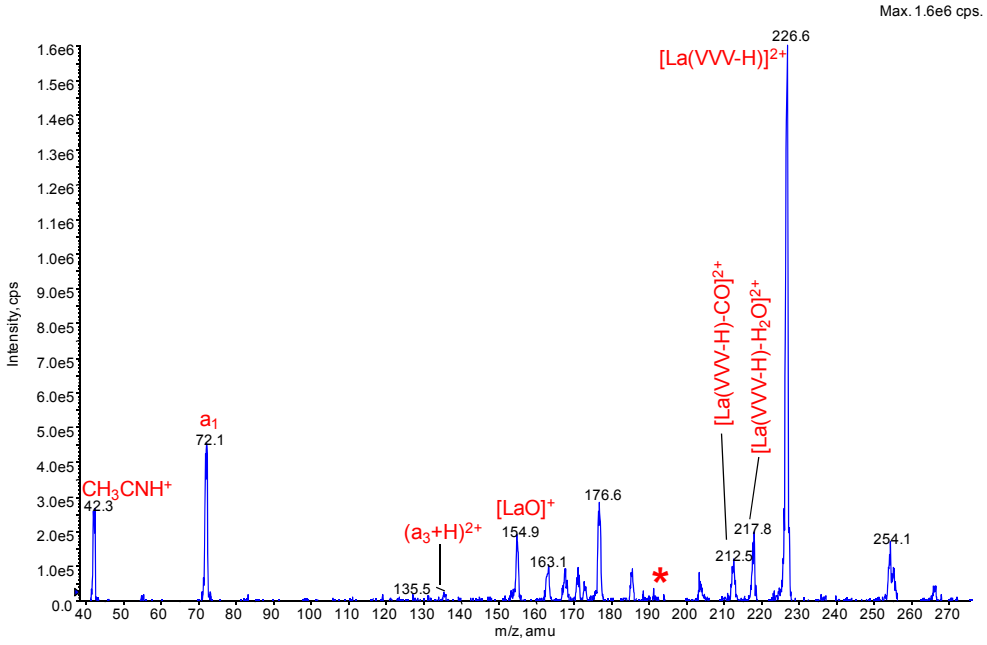

Figure S1b. CID of $[La(VVV)(CH_3CN)_3]^{3+}$ (*m/z* 192.2) at collision energy 51 eV.

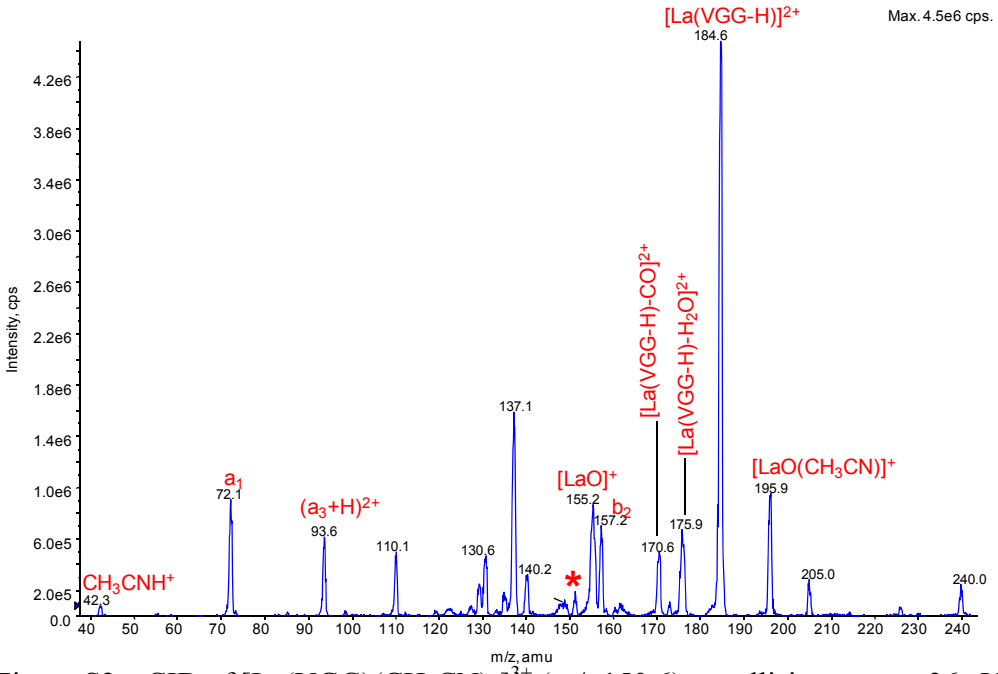

Figure S2a. CID of $[La(VGG)(CH_3CN)_2]^{3+}$ (*m/z* 150.6) at collision energy 36 eV.

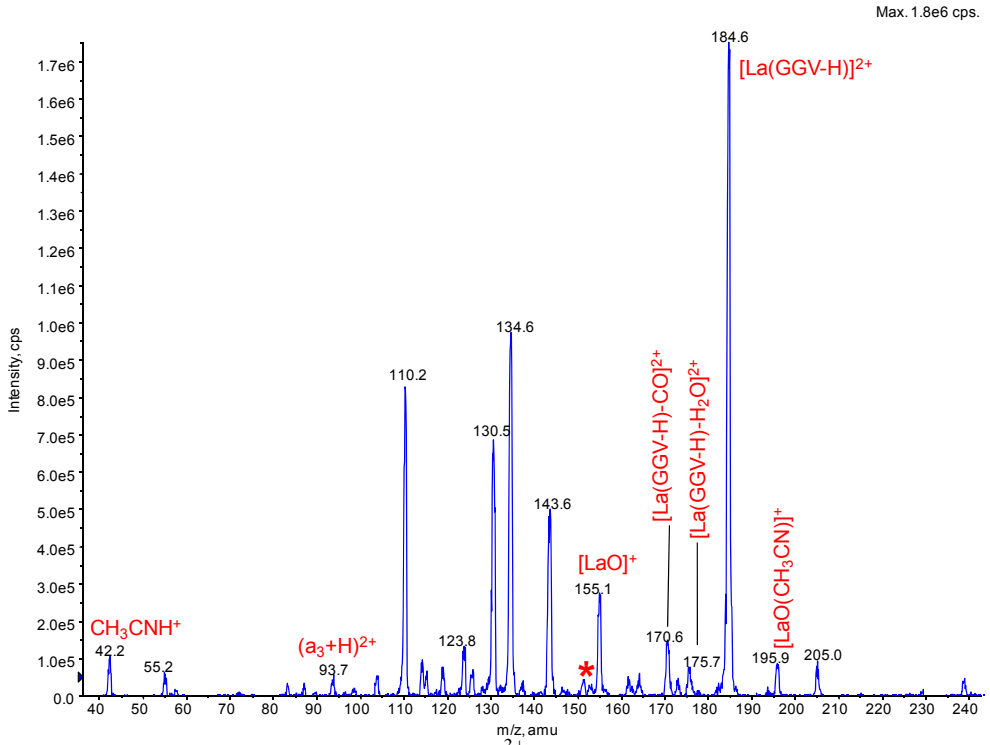

Figure S2b. CID of $[La(GGV)(CH_3CN)_2]^{3+}$ (*m/z* 150.6) at collision energy 36 eV.

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

linear a_2 of GG	Et = -303.0743456		
7	-1.841974	-0.885410	-0.008444
6	-1.411431	0.511628	0.010981
6	0.103181	0.639700	0.000367
8	0.776426	1.612037	-0.007869
7	0.773001	-0.716860	0.003835
6	2.038550	-0.863721	0.001329
1	-1.773622	1.086752	-0.847185
1	-1.755993	1.049796	0.899982
1	0.070662	-1.479388	0.006570
1	2.475034	-1.858262	0.004343
1	2.663588	0.028539	-0.004112
1	-2.409469	-1.123613	0.797276
1	-2.380598	-1.109874	-0.837730

linear $(a_2+H)^{2+}$ of GG	E_t= -303.2657948		
7	2.360025	0.080374	0.000241
6	1.128249	-0.787586	-0.000249
6	-0.099892	0.110825	-0.000082
8	-0.072393	1.293245	-0.000161
7	-1.411344	-0.599787	0.000059
6	-2.525769	0.049534	0.000110
1	2.402986	0.695601	-0.824597
1	2.403945	0.693250	0.826784
1	3.211780	-0.498474	-0.001071
1	1.154205	-1.426721	-0.888815
1	1.154083	-1.427567	0.887693
1	-1.433194	-1.623637	0.000164
1	-3.466596	-0.498234	0.000290
1	-2.504356	1.139080	0.000064

cyclic $(a_2+H)^{2+}$ of GG	E_t= -303.2661317		
7	1.426270	0.654691	-0.118503
6	0.029352	1.221834	0.096351
1	-0.045416	1.676390	1.089810
6	-0.828702	-0.020182	0.001747
8	-2.102636	-0.095755	-0.029103
7	-0.088845	-1.094810	-0.030595
6	1.349190	-0.860097	0.086559
1	1.720514	-1.116172	1.080942
1	-0.482718	-2.038293	-0.074690
1	-0.203260	1.969481	-0.665639
1	1.915202	-1.377474	-0.688450
1	1.756708	0.867352	-1.069368
1	-2.609898	0.738287	-0.028618
1	2.108934	1.077971	0.524586

a_2 of PP	Et= -536.6052256		
7	-2.371738	0.610504	-0.911292
6	-3.518567	-0.117595	-0.334794
6	-1.163420	-0.107748	-0.535973
6	-1.556954	-1.135800	0.613753
6	-2.996311	-0.726455	0.973903
6	-0.093976	0.828744	-0.068279
7	1.309807	0.251283	-0.062618
6	2.305849	0.951429	0.364403
6	3.602121	0.248472	0.252605
6	3.195349	-1.201973	-0.106175
6	1.736088	-1.085077	-0.592955
8	-0.206921	1.952548	0.306167
1	-3.833569	-0.902414	-1.029882
1	-4.360094	0.561809	-0.200799
1	-0.768198	-0.669303	-1.391740
1	-0.885414	-1.102485	1.475124
1	-1.525367	-2.147634	0.204902
1	-3.582174	-1.578266	1.324205
1	-2.992744	0.029161	1.764146
1	4.189359	0.346402	1.169868
1	4.190062	0.748828	-0.530691
1	3.248566	-1.835184	0.780013
1	3.838141	-1.639473	-0.867686
1	1.643182	-1.054518	-1.680554
1	1.078530	-1.859514	-0.203653
1	-2.342786	1.567102	-0.575466
1	2.130312	1.958608	0.731323

$(a_2+H)^{2+}$ of PP	Et= -536.858153		
7	-2.370041	0.615069	-0.850072
6	-3.549525	-0.059551	-0.136378
6	-1.120010	-0.217204	-0.584309
6	-1.558297	-1.259312	0.498226
6	-2.879040	-0.706416	1.065961
6	-0.042065	0.743143	-0.094433
7	1.329040	0.237872	-0.050899
6	2.296460	0.971619	0.427812
6	3.609045	0.326407	0.323932
6	3.291351	-1.122838	-0.116894
6	1.834740	-1.068523	-0.625084
8	-0.277913	1.856847	0.268805
1	-2.548102	0.735086	-1.851037
1	-3.967205	-0.789531	-0.830362
1	-4.295867	0.700482	0.089976
1	-0.818238	-0.696535	-1.516070
1	-0.803380	-1.394318	1.273921
1	-1.713047	-2.223995	0.012278

1	-3.497858	-1.497738	1.489677
1	-2.699660	0.029791	1.853864
1	4.171259	0.420533	1.260376
1	4.199515	0.902460	-0.409818
1	3.373723	-1.800495	0.732972
1	3.967278	-1.477593	-0.892601
1	1.760147	-1.001282	-1.712763
1	1.218938	-1.891652	-0.266361
1	-2.213847	1.555333	-0.457274
1	2.080708	1.960134	0.826598

a_3 of GGG	E_t= -511.1637153		
7	3.328879	-0.612255	-0.578381
6	2.714372	0.647930	-0.169229
6	1.258010	0.470214	0.238841
8	0.577412	1.435536	0.633832
7	0.771328	-0.777984	0.124560
6	-0.479150	-1.245029	0.706853
6	-1.738852	-0.734287	0.022211
7	-1.787940	0.760413	-0.032514
6	-2.818885	1.375497	-0.462096
1	4.083740	-0.893533	0.035421
1	3.693615	-0.577130	-1.522204
1	3.214739	1.110677	0.687112
1	2.729633	1.396739	-0.966165
1	-0.509211	-2.331759	0.661978
1	-0.543150	-0.942064	1.761137
8	-2.647792	-1.372030	-0.394392
1	-0.861217	1.236882	0.316761
1	1.460423	-1.449415	-0.220837
1	-2.824119	2.461257	-0.481386
1	-3.680252	0.803128	-0.802479

$(a_3+H)^{2+}$ of GGG	E_t= -511.4026113		
7	-4.141573	0.018789	-0.000252
6	-2.887705	0.855219	-0.000191
6	-1.719801	-0.153641	0.000086
8	-1.970366	-1.347279	-0.000164
7	-0.465529	0.346944	0.000475
6	0.669224	-0.559030	0.000541
6	1.947814	0.228904	0.000095
7	3.191386	-0.631043	-0.000121
6	4.364561	-0.110259	-0.000421
1	-4.725239	0.173805	-0.827091
1	-4.724750	0.173020	0.827092
1	-2.875576	1.488627	-0.887462
1	-2.875774	1.488798	0.886971
1	0.648656	-1.217625	0.880512

1	0.648094	-1.218222	-0.878904
8	2.080346	1.404296	-0.000013
1	3.093361	-1.648973	-0.000087
1	-0.286896	1.344599	0.000771
1	5.243045	-0.750689	-0.000628
1	4.452767	0.975006	-0.000462
1	-3.812066	-0.974457	-0.000669

a_3 of PPP	Et=-861.4506734		
6	2.855776	2.117472	-0.396195
6	2.572097	1.500389	0.970519
6	0.634660	1.082223	-0.531323
7	-1.859430	0.583270	-0.411951
6	-3.247711	1.055669	-0.167028
6	-4.091969	-0.193049	-0.403716
6	-3.200045	-1.320554	0.133212
6	-1.783260	-0.909706	-0.305082
6	-0.691670	-1.177268	0.729928
8	-0.783764	-0.740559	1.866955
7	0.524826	-1.619653	0.256458
6	1.696832	-0.936505	0.754743
6	0.809234	-2.442217	-0.937204
6	2.313364	-2.693451	-0.786568
6	2.830260	-1.372400	-0.186697
6	-0.850908	1.484613	-0.229478
8	-1.069754	2.637272	0.103527
6	1.458252	2.291258	-1.005759
7	1.372473	0.587977	0.745657
1	3.378994	3.068448	-0.291868
1	3.488146	1.464235	-1.000765
1	2.262099	2.256747	1.691905
1	3.386853	0.918126	1.398569
1	0.679143	0.264018	-1.245212
1	-3.471960	1.882944	-0.839788
1	-3.331176	1.422166	0.860190
1	-4.288408	-0.327875	-1.470887
1	-5.051816	-0.141983	0.110413
1	-3.465114	-2.307267	-0.248282
1	-3.239494	-1.347586	1.224493
1	-1.532083	-1.340177	-1.276635
1	1.898118	-1.148390	1.805773
1	0.587843	-1.909781	-1.870339
1	0.218104	-3.357289	-0.912928
1	2.793600	-2.934677	-1.734488
1	2.487124	-3.522521	-0.097508
1	2.972491	-0.640161	-0.983746
1	3.777798	-1.481946	0.339534
1	1.473886	2.342510	-2.094913

1	0.983658	3.198403	-0.631068
1	0.725780	0.688345	1.536427

$(a_3+H)^{2+}$ of PPP	E_t= -861.7260259		
6	-3.532440	-2.141180	1.235354
6	-4.391195	-1.693566	0.056534
6	-2.111410	-0.732625	-0.153708
7	-0.738583	1.383444	-0.074668
6	-0.620896	2.858152	-0.234345
6	0.372742	3.226930	0.859819
6	1.362509	2.051103	0.869947
6	0.502387	0.804509	0.442900
6	1.221949	-0.006229	-0.632826
8	0.838215	-0.204450	-1.741648
7	2.556617	-0.575375	-0.253030
6	3.390245	-0.956538	-1.170162
6	3.064737	-0.874042	1.135067
6	4.542824	-1.245243	0.891717
6	4.628481	-1.539951	-0.625450
1	-4.119432	-2.220365	2.150469
1	-3.086784	-3.120694	1.040593
1	-5.081637	-0.895405	0.328788
1	-4.940713	-2.486673	-0.447013
1	-1.309019	-1.363314	-0.534662
1	-3.185073	-1.723377	-1.693441
1	-1.602582	3.311551	-0.121118
1	-0.249394	3.091562	-1.236820
1	-0.137348	3.303938	1.822443
1	0.874035	4.175172	0.667123
1	1.823144	1.902938	1.845792
1	2.159452	2.225745	0.141818
1	3.126834	-0.845836	-2.218579
1	2.469829	-1.701538	1.528449
1	2.934323	-0.003956	1.773171
1	4.844895	-2.096810	1.498382
1	5.191070	-0.407172	1.148395
1	4.628156	-2.613296	-0.873280
1	5.512764	-1.133092	-1.126451
1	-1.574261	-1.380575	1.877221
1	-2.849045	-0.159803	1.816124
6	-1.879399	0.767264	-0.458250
8	-2.799585	1.372219	-0.996606
6	-2.452562	-1.050471	1.321867
7	-3.380517	-1.091456	-0.916786
1	0.318105	0.154440	1.305857
1	-3.706808	-0.180562	-1.306629