

Supporting Information for *Phys. Chem. Chem. Phys.*

Intramolecular Hydrogen Transfer in the Ionization Process of α -alanine

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- The Cartesian coordinates (\AA) for all stationary points and their electronic energies with ZPE correction (E_0), electronic and thermal energies (E), enthalpies (H) and free energies (G) at 298.15k and 1 atmosphere.

The Cartesian coordinates (Å) of conformer I at B3LYP/6-31++G(3df,2p) level.				The Cartesian coordinates (Å) of conformer I at G3B3 level.			
E ₀ = -323.694050 Hartree, E= -323.687077 Hartree				E ₀ = -323.532455 Hartree, E= -323.525368 Hartree			
H= -323.686133 Hartree, G= -323.724982 Hartree				H= -323.524423 Hartree G= -323.563559 Hartree			
C	-0.664410	0.142562	-0.399902	C	-0.671505	0.126507	-0.399520
C	-1.208467	1.262204	0.502004	C	-1.217569	1.275951	0.464120
C	0.779875	-0.167719	0.001816	C	0.781330	-0.166277	-0.013076
H	-1.251042	0.926109	1.542668	H	-1.219281	0.993951	1.524133
H	-2.220148	1.518038	0.182932	H	-2.247828	1.488508	0.166590
O	1.645218	0.770181	-0.457241	O	1.622174	0.829637	-0.389047
O	1.136716	-1.115121	0.659102	O	1.162643	-1.156473	0.572403
H	-0.579717	2.153242	0.451439	H	-0.612350	2.179478	0.349490
H	2.527957	0.524877	-0.140708	H	2.511253	0.566506	-0.083546
H	-0.639058	0.508701	-1.430939	H	-0.666300	0.455963	-1.445956
N	-1.543288	-1.017383	-0.346784	N	-1.537472	-1.040966	-0.290603
H	-1.229818	-1.733993	-0.994111	H	-1.189028	-1.777143	-0.903832
H	-1.502617	-1.438060	0.577807	H	-1.446243	-1.422899	0.651357

The Cartesian coordinates (Å) of conformer I cation at B3LYP/6-31++G(3df,2p) level.				The Cartesian coordinates (Å) of conformer I cation at G3B3 level.			
E ₀ = -323.373725 Hartree, E= -323.366631 Hartree				E ₀ = -323.198225 Hartree, E= -323.190990 Hartree			
H= -323.365687 Hartree, G= -323.405284 Hartree				H= -323.190046 Hartree, G= -323.229895 Hartree			
C	-0.708764	0.157924	0.375710	C	-0.708133	0.147159	0.380622
C	-1.676583	-0.937352	-0.034245	C	-1.671415	-0.943996	-0.062615
C	0.840135	-0.253625	0.022105	C	0.835137	-0.251064	0.027289
H	-1.717699	-1.047910	-1.120908	H	-1.698655	-1.037919	-1.153101
H	-2.673880	-0.702517	0.342003	H	-2.676027	-0.721478	0.306406
O	1.613590	0.817111	0.036461	O	1.597675	0.830889	0.007810
O	1.125775	-1.391547	-0.156766	O	1.141414	-1.394179	-0.126189
H	-1.353156	-1.888075	0.389615	H	-1.346754	-1.902090	0.349234
H	2.546137	0.570157	-0.105807	H	2.535776	0.581566	-0.139581
H	-0.605481	0.264959	1.467132	H	-0.633145	0.237640	1.476664
N	-0.972047	1.407900	-0.186647	N	-0.973065	1.410758	-0.161821
H	-0.537226	2.254514	0.168681	H	-0.543699	2.254678	0.214086
H	-1.498016	1.487375	-1.053167	H	-1.472285	1.506021	-1.045703

The Cartesian coordinates (Å) of conformer II at B3LYP/6-31++G(3df,2p) level. $E_0 = -323.692208$ Hartree, $E = -323.685273$ Hartree $H = -323.684329$ Hartree, $G = -323.722966$ Hartree				The Cartesian coordinates (Å) of conformer II at G3B3 level. $E_0 = -323.530754$ Hartree, $E = -323.523732$ Hartree $H = -323.522787$ Hartree, $G = -323.561601$ Hartree			
C	-0.653286	0.159503	-0.411093	C	-0.655303	0.161707	-0.415948
C	-1.202485	1.235054	0.552672	C	-1.204971	1.230098	0.558098
C	0.775499	-0.165844	-0.009263	C	0.774840	-0.163927	-0.012817
H	-1.211109	0.860612	1.580249	H	-1.205663	0.847850	1.585396
H	-2.227959	1.487004	0.268669	H	-2.235603	1.483225	0.284186
O	1.654888	0.747612	-0.481569	O	1.657849	0.743799	-0.490243
O	1.107783	-1.096418	0.683700	O	1.101810	-1.088635	0.698486
H	-0.604993	2.149984	0.513858	H	-0.609906	2.149566	0.526611
H	2.529639	0.501545	-0.144403	H	2.530680	0.485722	-0.137492
H	-0.620341	0.585651	-1.418990	H	-0.627396	0.594973	-1.422918
N	-1.414166	-1.086026	-0.448726	N	-1.404655	-1.090994	-0.458680
H	-1.175143	-1.663653	0.352084	H	-1.180326	-1.635233	0.373101
H	-2.410666	-0.900788	-0.421342	H	-2.403864	-0.897730	-0.440067

The Cartesian coordinates (Å) of conformer II cation at B3LYP/6-31++G(3df,2p) level. $E_0 = -323.369083$ Hartree, $E = -323.362088$ Hartree $H = -323.361144$ Hartree, $G = -323.400630$ Hartree				The Cartesian coordinates (Å) of conformer II cation at G3B3 level. $E_0 = -323.199831$ Hartree, $E = -323.192715$ Hartree $H = -323.191771$ Hartree, $G = -323.231609$ Hartree			
C	-0.645058	0.120385	-0.422754	C	0.651430	-0.105548	-0.413709
C	-1.318092	1.232321	0.489767	C	1.342212	-1.232011	0.456584
C	0.817727	-0.132278	-0.021152	C	-0.820965	0.123127	-0.027416
H	-1.242362	0.946013	1.538653	H	1.267670	-0.983583	1.517098
H	-2.360842	1.369963	0.203839	H	2.387958	-1.352284	0.165471
O	1.586816	0.892181	-0.346761	O	-1.557942	-0.939063	-0.307809
O	1.140513	-1.153586	0.529287	O	-1.178200	1.162618	0.477142
H	-0.759603	2.150034	0.300417	H	0.795744	-2.154307	0.244365
H	2.508068	0.720579	-0.084124	H	-2.488552	-0.772454	-0.051003
H	-0.754131	0.472763	-1.458402	H	0.765220	-0.417214	-1.464898
N	-1.320956	-1.110505	-0.267258	N	1.300607	1.140735	-0.227428
H	-0.818367	-1.856318	0.237518	H	0.755144	1.878197	0.250599

H	-2.272160	-1.260824	-0.602469	H	2.265640	1.314659	-0.517057
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The Cartesian coordinates (Å) of conformer III at B3LYP/6-31++G(3df,2p) level. E ₀ = -323.692189 Hartree, E= -323.685227 Hartree H= -323.684283 Hartree, G= -323.723390 Hartree				The Cartesian coordinates (Å) of conformer III at G3B3 level. E ₀ = -323.530492 Hartree, E= -323.523390 Hartree H= -323.522446 Hartree, G= -323.563371 Hartree			
C	-0.746252	0.273159	0.169586	C	-0.743952	0.256230	0.166210
C	-0.676119	0.137554	1.696627	C	-0.704482	0.188249	1.701942
C	0.672731	0.292447	-0.401724	C	0.697093	0.272795	-0.355614
H	-0.265261	-0.835972	1.979218	H	-0.266381	-0.760109	2.036490
H	-1.683266	0.221110	2.109287	H	-1.724651	0.250887	2.090337
O	1.209306	-0.951508	-0.501025	O	1.110084	-0.946422	-0.793671
O	1.281433	1.284727	-0.721352	O	1.422200	1.242756	-0.359318
H	-0.047098	0.917512	2.132378	H	-0.107383	1.007476	2.112568
H	2.108894	-0.844136	-0.844190	H	2.041206	-0.830388	-1.062334
H	-1.165510	1.250409	-0.080994	H	-1.164742	1.225853	-0.123064
N	-1.627878	-0.753121	-0.384363	N	-1.614048	-0.792357	-0.357141
H	-1.736405	-0.641935	-1.387337	H	-1.651810	-0.740236	-1.373907
H	-1.244291	-1.679855	-0.225742	H	-1.212849	-1.704341	-0.142129

The Cartesian coordinates (Å) of conformer III cation at B3LYP/6-31++G(3df,2p) level. E ₀ = -323.372674 Hartree, E= -323.365517 Hartree H= -323.364573 Hartree, G= -323.404401 Hartree				The Cartesian coordinates (Å) of conformer III cation at G3B3 level. E ₀ = -323.197006 Hartree, E= -323.189696 Hartree H= -323.188752 Hartree, G= -323.228959 Hartree			
C	0.727841	-0.168244	-0.442171	C	0.722571	-0.169834	-0.443299
C	1.290933	-1.134267	0.620320	C	1.294618	-1.136926	0.617912
C	-0.865532	-0.051612	-0.110834	C	-0.862150	-0.051309	-0.112556
H	1.217673	-0.713732	1.625894	H	1.209554	-0.723967	1.627586
H	2.339161	-1.329726	0.386610	H	2.347567	-1.322728	0.389532
O	-1.102833	0.940578	0.728932	O	-1.096322	0.949339	0.722582
O	-1.620698	-0.836721	-0.584189	O	-1.625966	-0.844822	-0.573866
H	0.736113	-2.072265	0.581476	H	0.747191	-2.081350	0.569934
H	-2.046952	0.964506	0.972131	H	-2.047268	0.970353	0.965940
H	0.768314	-0.576357	-1.451459	H	0.774142	-0.577808	-1.453787
N	1.287016	1.110128	-0.412496	N	1.284485	1.111771	-0.411006
H	1.400079	1.660702	-1.258709	H	1.406903	1.665088	-1.257636
H	1.445294	1.589861	0.469687	H	1.418586	1.600289	0.473410

The Cartesian coordinates (Å) of conformer IV at B3LYP/6-31++G(3df,2p) level.				The Cartesian coordinates (Å) of conformer IV at G3B3 level.			
E ₀ = -323.693305 Hartree, E= -323.686619 Hartree				E ₀ = -323.531667 Hartree, E= -323.524911 Hartree			
H= -323.685674 Hartree, G= -323.723779 Hartree				H= -323.523966 Hartree, G= -323.562185 Hartree			
C	-0.623828	0.167632	-0.423901	C	-0.727804	0.254513	0.101994
C	-1.257478	1.228259	0.482111	C	-0.736509	0.314349	1.633852
C	0.876476	0.048731	-0.087577	C	0.735850	0.292598	-0.391366
H	-1.243328	0.902506	1.526781	H	-0.269952	-0.582650	2.057399
H	-2.294977	1.410860	0.187506	H	-1.762301	0.387338	2.013780
O	1.208272	-1.076049	0.564428	O	1.186093	-0.888093	-0.842189
O	1.676046	0.904527	-0.367896	O	1.414132	1.291475	-0.338667
H	-0.704573	2.165021	0.405120	H	-0.175542	1.188407	1.973218
H	0.375500	-1.593046	0.630858	H	0.404399	-1.494492	-0.775250
H	-0.672916	0.513492	-1.461707	H	-1.211319	1.158626	-0.289531
N	-1.279584	-1.140576	-0.240517	N	-1.365704	-0.986392	-0.379710
H	-2.227394	-1.041656	0.104224	H	-2.066205	-1.322285	0.276884
H	-1.320789	-1.668697	-1.105217	H	-1.835145	-0.836792	-1.270300

The Cartesian coordinates (Å) of conformer IV/V cation at B3LYP/6-31++G(3df,2p) level.				The Cartesian coordinates (Å) of conformer IV/V cation at G3B3 level.			
E ₀ = -323.361690 Hartree, E= -323.354336 Hartree				E ₀ = -323.185814 Hartree, E= -323.178448 Hartree			
H= -323.353392 Hartree, G= -323.393477 Hartree				H= -323.177503 Hartree, G= -323.217471 Hartree			
C	0.799519	-0.054829	-0.416589	C	-0.843684	0.243235	0.157842
C	1.377470	-1.180264	0.420197	C	-0.805804	0.416135	1.669674
C	-0.973248	-0.089437	-0.058183	C	0.845220	0.182946	-0.350317
H	1.342100	-0.957011	1.490526	H	-0.411125	-0.470680	2.177660
H	2.423105	-1.317797	0.128952	H	-1.826696	0.596870	2.022830
O	-1.481622	1.012254	0.404183	O	1.196680	-0.846202	-1.063028
O	-1.495874	-1.120832	-0.291494	O	1.508946	1.104654	0.003238
H	0.832626	-2.105168	0.235498	H	-0.180159	1.272521	1.929232
H	-0.812802	1.711734	0.501062	H	0.442193	-1.458379	-1.192238
H	0.705248	-0.259961	-1.484903	H	-1.137183	1.138547	-0.398701
N	1.283752	1.204598	-0.174353	N	-1.489829	-0.881277	-0.315228
H	1.780597	1.412352	0.685542	H	-1.677527	-1.666165	0.305236
H	1.340383	1.899459	-0.910271	H	-2.031038	-0.855603	-1.176085

The Cartesian coordinates (Å) of conformer V at B3LYP/6-31++G(3df,2p) level.				The Cartesian coordinates (Å) of conformer V at G3B3 level.			
E ₀ = -323.693163 Hartree, E= -323.686477 Hartree				E ₀ = -323.531212 Hartree, E= -323.524510 Hartree			
H= -323.685533 Hartree, G= -323.723771 Hartree				H= -323.523566 Hartree, G= -323.561551 Hartree			
C	-0.643626	-0.035669	0.379661	C	-0.647034	0.001343	0.376605
C	-1.420621	-1.188271	-0.259659	C	-1.471095	-1.151590	-0.199539
C	0.865359	-0.137807	0.059356	C	0.857208	-0.166584	0.053665
H	-1.415346	-1.096467	-1.350790	H	-1.463468	-1.122855	-1.296168
H	-2.458602	-1.185055	0.082855	H	-2.510750	-1.095017	0.140808
O	1.443670	1.036652	-0.231027	O	1.495005	0.996003	-0.151819
O	1.475164	-1.175865	0.096614	O	1.410099	-1.240902	0.024099
H	-0.963304	-2.144335	-0.002241	H	-1.046044	-2.109438	0.109555
H	0.716203	1.696940	-0.198818	H	0.785195	1.684964	-0.098824
H	-0.699628	-0.129112	1.469520	H	-0.707187	-0.028103	1.472906
N	-1.134410	1.310876	0.025805	N	-1.069886	1.356143	-0.033856
H	-1.589684	1.308273	-0.881723	H	-1.407023	1.343687	-0.996144
H	-1.806113	1.657812	0.699716	H	-1.836826	1.693939	0.542235

The Cartesian coordinates (Å) of TS-44-1 at B3LYP/6-31++G(3df,2p) level.				The Cartesian coordinates (Å) of TS-44-1 at G3B3 level.			
E ₀ = -323.366168 Hartree, E= -323.358690 Hartree				E ₀ = -323.192453 Hartree, E= -323.184458 Hartree			
H= -323.357746 Hartree, G= -323.399262 Hartree				H= -323.183514 Hartree, G= -323.226532 Hartree			
C	1.129222	-0.084339	0.424812	C	1.357974	-0.128126	0.423825
C	1.608162	1.177692	-0.197199	C	1.688546	1.204096	-0.126737
C	-1.170997	0.152032	0.030111	C	-1.338626	0.103906	0.029544
H	1.746403	1.084210	-1.276380	H	2.025633	1.164313	-1.165834
H	2.579552	1.415701	0.257546	H	2.489127	1.634376	0.493933
O	-1.631108	-1.059572	-0.110394	O	-1.955029	-1.051911	-0.033716
O	-1.610667	1.242567	0.031549	O	-1.679917	1.239547	-0.042592
H	0.935032	2.006200	0.021156	H	0.827652	1.874188	-0.037531
H	-2.601380	-1.068090	-0.247990	H	-2.925182	-0.933893	-0.168839
H	0.821797	-0.082760	1.467009	H	0.949532	-0.212641	1.427757
N	1.429620	-1.260133	-0.078006	N	1.691602	-1.243159	-0.155732
H	1.227587	-2.119325	0.418764	H	1.510801	-2.147496	0.273747
H	1.819544	-1.351272	-1.009654	H	2.113436	-1.257073	-1.082434

The Cartesian coordinates (Å) of TS-44-2 at B3LYP/6-31++G(3df,2p) level.				The Cartesian coordinates (Å) of TS-44-2 at G3B3 level.			
E ₀ = -323.365743 Hartree, E= -323.358351 Hartree				E ₀ = -323.190152 Hartree, E= -323.182548 Hartree			
H= -323.357406 Hartree, G= -323.398514 Hartree				H= -323.181603 Hartree, G= -323.223110 Hartree			
C	-1.046524	0.153766	-0.436360	C	-1.102272	0.084378	-0.435438
C	-1.338945	1.200574	0.588209	C	-1.390651	1.264267	0.433471
C	1.109124	-0.172766	0.043766	C	1.142896	-0.166968	0.017238
H	-1.447231	0.778135	1.589613	H	-1.501461	0.989395	1.486637
H	-2.289958	1.675366	0.311235	H	-2.339661	1.703498	0.090947
O	1.738915	0.807168	-0.532641	O	1.717399	0.954147	-0.320323
O	1.370542	-1.112558	0.697229	O	1.475497	-1.217842	0.442465
H	-0.578551	1.980802	0.593685	O	-0.622185	2.032278	0.329889
H	2.707009	0.762147	-0.385823	H	2.694128	0.919874	-0.184328
H	-0.717246	0.456402	-1.427519	H	-0.790189	0.246576	-1.465514
N	-1.612852	-1.034196	-0.363003	N	-1.617624	-1.098022	-0.175778
H	-2.046407	-1.360144	0.493395	H	-2.020713	-1.313484	0.732485
H	-1.555235	-1.699657	-1.123958	H	-1.539560	-1.872487	-0.828430

The Cartesian coordinates (Å) of TS-44-4 at B3LYP/6-31++G(3df,2p) level.				The Cartesian coordinates (Å) of TS-44-4 at G3B3 level.			
E ₀ = -323.360551 Hartree, E= -323.353172 Hartree				E ₀ = -323.183903 Hartree, E= -323.176322 Hartree			
H= -323.352228 Hartree, G= -323.393075 Hartree				H= -323.175378 Hartree, G= -323.216709 Hartree			
C	-0.173215	-0.024715	0.035141	C	1.149788	-0.035079	-0.414595
C	0.001295	-0.032613	1.513242	C	1.476964	-1.173207	0.488738
C	2.080179	0.044731	-0.550075	C	-1.222985	-0.065139	-0.052235
H	0.206275	-1.031205	1.906262	H	1.581775	-0.867298	1.534169
H	-0.944667	0.317757	1.950224	H	2.441575	-1.585807	0.154532
O	2.542652	-0.941667	-1.267857	O	-1.841789	0.998878	0.397890
O	2.570232	1.027449	-0.139734	O	-1.623352	-1.125378	-0.381461
H	0.780626	0.660917	1.825493	H	0.735326	-1.968886	0.404764
H	1.880551	-1.628694	-1.439673	H	-1.227041	1.727740	0.600346
H	-0.194564	0.923550	-0.493224	H	0.833220	-0.238293	-1.434339
N	-0.738629	-1.043152	-0.591098	O	1.609154	1.180944	-0.186662
H	-0.928372	-1.916049	-0.111276	H	2.076021	1.415703	0.685954
H	-1.085022	-0.957062	-1.539085	H	1.593570	1.902785	-0.901676

The Cartesian coordinates (Å) of TS1-2 at B3LYP/6-31++G(3df,2p) level. E ₀ = -323.367582 Hartree, E= -323.360983 Hartree H= -323.360039 Hartree, G= -323.398346 Hartree				The Cartesian coordinates (Å) of TS1-2 at G3B3 level. E ₀ = -323.195725 Hartree, E= -323.189000 Hartree H= -323.188056 Hartree, G= -323.226569 Hartree			
C	-0.662520	0.166285	-0.457166	C	-0.663000	0.170116	-0.458473
C	-1.233559	1.212397	0.579828	C	-1.237178	1.210158	0.581192
C	0.813923	-0.137244	0.052505	C	0.813828	-0.136979	0.049830
H	-1.227909	0.792657	1.585865	H	-1.223428	0.789967	1.589051
H	-2.247799	1.473835	0.277672	H	-2.256385	1.469389	0.286751
O	1.666392	0.562181	-0.674085	O	1.667330	0.565458	-0.675001
O	1.018877	-0.875270	0.967732	O	1.017349	-0.876487	0.971351
H	-0.594392	2.095410	0.535809	H	-0.603027	2.099363	0.537617
H	2.576834	0.415768	-0.358807	H	2.580025	0.415061	-0.348257
H	-0.655540	0.585953	-1.462031	H	-0.656508	0.590110	-1.464674
N	-1.372186	-1.041953	-0.444304	N	-1.368406	-1.043895	-0.447558
H	-1.306065	-1.658624	0.367708	H	-1.297335	-1.661184	0.366243
H	-1.929045	-1.355253	-1.236264	H	-1.923831	-1.366987	-1.239912

The Cartesian coordinates (Å) of TS2-2 at B3LYP/6-31++G(3df,2p) level. E ₀ = -323.353435 Hartree, E= -323.346291 Hartree H= -323.345347 Hartree, G= -323.385049 Hartree				The Cartesian coordinates (Å) of TS2-2 at G3B3 level. E ₀ = -323.177395 Hartree, E= -323.170137 Hartree H= -323.169193 Hartree, G= -323.209062 Hartree			
C	-0.744380	0.170743	0.368629	C	-0.737017	0.157329	0.368669
C	-1.665693	-0.957916	-0.041105	C	-1.661024	-0.963243	-0.070856
C	0.909332	-0.256304	-0.007565	C	0.902678	-0.252719	-0.005938
H	-1.737119	-1.045111	-1.128510	H	-1.722674	-1.033979	-1.161943
H	-2.662082	-0.765813	0.364460	H	-2.662483	-0.780747	0.330704
O	1.749764	0.761801	0.105763	O	1.736171	0.778478	0.076200
O	1.118285	-1.405328	-0.146067	O	1.131957	-1.408840	-0.110788
H	-1.299128	-1.904234	0.354103	H	-1.294443	-1.917684	0.310950
H	1.843099	1.304581	-0.693413	H	1.807300	1.299982	-0.746327
H	-0.557842	0.249777	1.449249	H	-0.576679	0.217307	1.456406
N	-1.033745	1.403045	-0.168825	N	-1.031706	1.405674	-0.141062
H	-1.594419	1.485665	-1.010616	H	-1.597535	1.510433	-0.980476
H	-0.696241	2.262895	0.249179	H	-0.704391	2.259670	0.303582

The Cartesian coordinates (Å) of INT-2 at B3LYP/6-31++G(3df,2p) level. $E_0 = -323.373725$ Hartree, $E = -323.366631$ Hartree $H = -323.365687$ Hartree, $G = -323.405283$ Hartree	The Cartesian coordinates (Å) of INT-2 at G3B3 level. $E_0 = -323.198225$ Hartree, $E = -323.190990$ Hartree $H = -323.190043$ Hartree, $G = -323.229896$ Hartree
C -0.708755 0.157891 0.375761	C 0.693826 0.202748 -0.435695
C -1.676612 -0.937307 -0.034333	C 1.627292 -0.990393 -0.293804
C 0.840138 -0.253632 0.022088	C -0.857046 -0.227864 -0.161497
H -1.717925 -1.047565 -1.121015	H 1.664288 -1.351625 0.739081
H -2.673854 -0.702683 0.342198	H 2.634054 -0.711527 -0.615664
O 1.613559 0.817098 0.036384	O -1.584699 0.836191 0.139639
O 1.125755 -1.391585 -0.156679	O -1.197411 -1.364480 -0.289362
H -1.353039 -1.888117 0.389227	H 1.267670 -1.807586 -0.922958
H 2.546118 0.570170 -0.105865	H -2.528394 0.584160 0.239166
H -0.605543 0.264917 1.467167	H 0.608539 0.563177 -1.473880
N -0.971966 1.407932 -0.186596	N 1.004853 1.285252 0.396350
H -1.498012 1.487428 -1.053068	H 1.516253 1.145178 1.267202
H -0.537123 2.254508 0.168793	H 0.599082 2.207815 0.247769

The Cartesian coordinates (Å) of INT-44-1 at B3LYP/6-31++G(3df,2p) level. $E_0 = -323.369464$ Hartree, $E = -323.361093$ Hartree $H = -323.360149$ Hartree, $G = -323.405643$ Hartree	The Cartesian coordinates (Å) of INT-44-1 at G3B3 level. $E_0 = -323.199270$ Hartree, $E = -323.190052$ Hartree $H = -323.189108$ Hartree, $G = -323.236510$ Hartree
C -0.745364 -0.290089 0.152826	C -1.692949 0.106137 0.399292
C -0.080142 -0.112172 1.445741	C -2.067249 -1.206281 -0.154813
C 2.491895 0.231368 -1.291036	C 1.930659 0.357354 0.014171
H -0.285778 -0.911321 2.158566	H -2.614594 -1.138927 -1.098098
H -0.374902 0.859302 1.862452	H -2.670145 -1.747129 0.587285
O 3.152268 0.348350 -2.413469	O 3.203761 0.090507 -0.107620
O 2.812286 0.284373 -0.145218	O 0.969590 -0.362596 0.096867
H 0.998309 -0.033290 1.247378	H -1.147347 -1.788167 -0.292861
H 4.103771 0.522939 -2.255689	H 3.369890 -0.880776 -0.131474
H -0.612898 0.459462 -0.624759	H -1.151960 0.159211 1.339773
N -1.487790 -1.300213 -0.151142	N -1.996450 1.232812 -0.154873
H -1.921341 -1.387770 -1.065477	H -1.722756 2.123740 0.254942
H -1.661080 -2.051744 0.511755	H -2.497509 1.275808 -1.041338

The Cartesian coordinates (Å) of INT-44-2 at B3LYP/6-31++G(3df,2p) level.				The Cartesian coordinates (Å) of INT-44-2 at G3B3 level.			
E ₀ = -323.380469 Hartree, E= -323.372394 Hartree				E ₀ = -323.205259 Hartree, E= -323.197092 Hartree			
H= -323.371450 Hartree, G= -323.415251 Hartree				H= -323.196147 Hartree, G= -323.240155 Hartree			
C	-2.057616	-0.343287	0.002207	C	-2.059922	-0.346727	0.000831
C	-3.529547	-0.332468	-0.000942	C	-3.535435	-0.333892	0.000087
C	2.275149	-0.379291	-0.001368	C	2.271861	-0.384546	-0.001582
H	-3.952521	0.672638	-0.009951	H	-3.959032	0.673202	-0.003235
H	-3.887881	-0.883396	0.877229	H	-3.896295	-0.886953	0.878241
O	3.570715	-0.386228	-0.002742	O	3.572737	-0.396201	-0.001844
O	1.475538	0.516459	0.004755	O	1.488279	0.533648	0.004046
H	-3.882793	-0.898381	-0.871559	H	-3.895487	-0.892385	-0.874914
H	3.960071	0.513012	0.003784	H	3.946827	0.516170	0.003860
H	-1.534383	-1.298951	0.007300	H	-1.534444	-1.301882	0.004440
N	-1.313866	0.702540	-0.002046	N	-1.315052	0.701674	-0.002250
H	-1.723008	1.633844	-0.007274	H	-1.724788	1.635756	-0.005651
H	-0.280364	0.631877	-0.000688	H	-0.278581	0.635795	-0.000638

The Cartesian coordinates (Å) of INT-44-4 at B3LYP/6-31++G(3df,2p) level.				The Cartesian coordinates (Å) of INT-44-4 at G3B3 level.			
E ₀ = -323.385954 Hartree, E= -323.377033 Hartree				E ₀ = -323.210720 Hartree, E= -323.201693 Hartree			
H= -323.376088 Hartree, G= -323.422310 Hartree				H= -323.200749 Hartree, G= -323.247334 Hartree			
C	2.059718	-0.323085	0.000070	C	-2.006411	-0.297067	-0.003680
C	3.531823	-0.344613	-0.000876	C	-3.477858	-0.406341	0.005972
C	-2.509112	0.357206	0.000781	C	2.474406	0.353163	0.017077
H	3.976666	0.651124	-0.006736	H	-3.984707	0.561552	0.008245
H	3.876236	-0.915564	-0.871824	H	-3.784640	-0.988986	0.885501
O	-3.512804	-0.487392	-0.002709	O	3.479908	-0.496380	-0.006730
O	-1.345949	0.082836	0.005280	O	1.307505	0.066493	-0.005187
H	3.876576	-0.904795	0.876970	H	-3.796940	-0.991477	-0.867397
H	-4.361590	-0.017972	-0.007627	H	4.329529	-0.017921	0.018234
H	1.507992	-1.262133	0.002845	H	-1.396827	-1.200728	-0.007683
N	1.344235	0.742986	-0.001429	N	-1.351487	0.810041	-0.006301
H	1.777167	1.662530	-0.004200	H	-1.829870	1.710081	-0.003614
H	0.312766	0.685313	0.000160	H	-0.316262	0.797753	-0.010063

The Cartesian coordinates (Å) of COOH-1 at B3LYP/6-31++G(3df,2p) level. E ₀ = -189.103510 Hartree, E= -189.100304 Hartree H= -189.099360 Hartree, G= -189.127945 Hartree	The Cartesian coordinates (Å) of COOH-1 at G3B3 level. E ₀ = -189.002111 Hartree, E= -188.998892 Hartree H= -188.997947 Hartree, G= -189.026570 Hartree
C -0.133369 -0.419269 0.000000 O 1.119363 0.016884 0.000000 O -1.160259 0.173240 0.000000 H 1.127382 0.994625 0.000000	C 0.000000 0.447056 0.000000 O -1.065566 -0.349850 0.000000 O 1.161036 0.175409 0.000000 H -0.763758 -1.286811 0.000000

The Cartesian coordinates (Å) of COOH-2 at B3LYP/6-31++G(3df,2p) level. E ₀ = -189.106143 Hartree, E= -189.102923 Hartree H= -189.101979 Hartree, G= -189.130529 Hartree	The Cartesian coordinates (Å) of COOH-2 at G3B3 level. E ₀ = -189.004858 Hartree, E= -189.001611 Hartree H= -189.000667 Hartree, G= -189.029278 Hartree
C 0.132096 0.388056 -0.000087 O -1.068895 -0.212332 -0.000038 O 1.189387 -0.137025 0.000051 H -1.756511 0.466518 0.000418	C -0.131556 0.394759 0.000000 O 1.071136 -0.215632 0.000000 O -1.192280 -0.139411 0.000000 H 1.758483 0.471786 0.000002

The Cartesian coordinates (Å) of COOH⁺ at B3LYP/6-31++G(3df,2p) level. E ₀ = -188.802137 Hartree, E= -188.798920 Hartree H= -188.797976 Hartree, G= -188.825163 Hartree	The Cartesian coordinates (Å) of COOH⁺ at G3B3 level. E ₀ = -188.708342 Hartree, E= -188.705046 Hartree H= -188.704102 Hartree, G= -188.731419 Hartree
C 0.000000 0.109860 0.000000 O 0.001467 -1.111486 0.000000 O -0.108041 1.230796 0.000000 H 0.852594 -1.613641 0.000000	C 0.000000 0.110351 0.000000 O 0.065510 -1.113963 0.000000 O -0.183684 1.228299 0.000000 H 0.945395 -1.576793 0.000000

The Cartesian coordinates (Å) of $\text{CH}_3\text{CHNH}_2^+$ at B3LYP/6-31++G(3df,2p) level.				The Cartesian coordinates (Å) of $\text{CH}_3\text{CHNH}_2^+$ at G3B3 level.			
E ₀ = -134.256812 Hartree, E= -134.252748 Hartree H= -134.251804 Hartree, G= -134.281874 Hartree				E ₀ = -134.182102 Hartree, E= -134.177961 Hartree H= -134.177017 Hartree, G= -134.207232 Hartree			
C	-0.082544	0.453308	-0.000067	C	-0.083200	0.454948	-0.000017
C	1.246648	-0.170653	0.000007	C	1.249402	-0.170065	-0.000002
H	1.216018	-1.260680	-0.000245	H	1.220787	-1.262125	-0.000186
H	1.803072	0.193583	0.873672	H	1.808026	0.190969	0.875722
H	1.803460	0.193963	-0.873253	H	1.808231	0.191283	-0.875457
H	-0.167221	1.539098	0.000047	H	-0.168667	1.541680	0.000008
N	-1.191288	-0.202005	0.000024	N	-1.193456	-0.202278	0.000001
H	-1.210233	-1.219467	-0.000067	H	-1.213054	-1.222737	-0.000011
H	-2.090710	0.271610	0.000038	H	-2.098341	0.267579	0.000033

The Cartesian coordinates (Å) of CH_3CHNH_2 at B3LYP/6-31++G(3df,2p) level.				The Cartesian coordinates (Å) of CH_3CHNH_2 at G3B3 level.			
E ₀ = -134.469675 Hartree, E= -134.465081 Hartree H= -134.464137 Hartree, G= -134.495810 Hartree				E ₀ = -134.391330 Hartree, E= -134.386718 Hartree H= -134.385773 Hartree, G= -134.417498 Hartree			
C	-0.058653	0.520823	-0.117029	C	-0.062777	0.520078	-0.126121
C	1.252743	-0.176609	0.016130	C	1.251789	-0.175913	0.015016
H	1.306678	-1.061432	-0.632430	H	1.299994	-1.078517	-0.613031
H	1.448400	-0.527353	1.044567	H	1.461734	-0.501359	1.050365
H	2.073331	0.487328	-0.265981	H	2.071474	0.481067	-0.294636
H	-0.139670	1.568324	0.153328	H	-0.139467	1.560366	0.184053
N	-1.222212	-0.230892	0.103100	N	-1.225422	-0.234280	0.118792
H	-1.210935	-1.160574	-0.298803	H	-1.209970	-1.153091	-0.316985
H	-2.086864	0.244665	-0.116984	H	-2.083746	0.245421	-0.134683

The Cartesian coordinates (Å) of $\text{CH}_3\text{CHNH}_3^+$ at B3LYP/6-31++G(3df,2p) level.				The Cartesian coordinates (Å) of $\text{CH}_3\text{CHNH}_3^+$ at G3B3 level.			
E ₀ = -134.794535 Hartree, E= -134.789411 Hartree H= -134.788467 Hartree, G= -134.821702 Hartree				E ₀ = -134.717681 Hartree, E= -134.712537 Hartree H= -134.711593 Hartree, G= -134.744828 Hartree			
C	-0.057761	0.560296	-0.060390	C	-0.058352	0.560204	-0.068835
C	-1.315805	-0.205573	0.006264	C	-1.318602	-0.206388	0.007736
H	-1.486439	-0.639337	1.005144	H	-1.496740	-0.622634	1.014514
H	-1.339472	-1.031152	-0.715820	H	-1.345716	-1.042436	-0.704270
H	-2.155592	0.458301	-0.205323	H	-2.156967	0.458136	-0.218222
H	1.430199	-0.537503	0.955863	H	1.450317	-0.507183	0.966635
H	0.059385	1.616684	0.138823	H	0.056296	1.612991	0.158363
N	1.218462	-0.194518	0.005999	N	1.221583	-0.193689	0.006971
H	1.192738	-1.018815	-0.606797	H	1.188750	-1.040508	-0.579143
H	2.011341	0.385109	-0.289131	H	2.014706	0.374566	-0.320079

The Cartesian coordinates (Å) of CH_3CHNH_3 at B3LYP/6-31++G(3df,2p) level.				The Cartesian coordinates (Å) of CH_3CHNH_3 at G3B3 level.			
E ₀ = -135.007227 Hartree, E= -135.002705 Hartree H= -135.001761 Hartree, G= -135.032775 Hartree				E ₀ = -134.932104 Hartree, E= -134.927544 Hartree H= -134.926600 Hartree, G= -134.957654 Hartree			
C	-0.061527	0.679886	-0.192027	C	-0.064344	0.690475	-0.191203
C	-1.256162	-0.226585	0.015966	C	-1.248412	-0.228325	0.016389
H	-1.395417	-0.941045	-0.807302	H	-1.387352	-0.940234	-0.815478
H	-2.165960	0.379478	0.054283	H	-2.165112	0.372283	0.056617
H	-1.234643	-0.829533	0.957401	H	-1.237666	-0.850150	0.950584
H	0.004229	1.392939	0.639842	H	-0.001360	1.377042	0.668498
N	1.175184	-0.206907	0.015080	N	1.169272	-0.204933	0.014545
H	2.008217	0.377345	0.015368	H	2.011077	0.372213	0.000361
H	1.260423	-0.836824	-0.780168	H	1.241513	-0.839164	-0.783475
H	1.202993	-0.813819	0.871384	H	1.230530	-0.830363	0.869961