

Supporting Information

Lifetimes and Stabilities of familiar explosives molecular adduct complexes during ion mobility measurements

Alan Mckenzie¹, John Daniel DeBord¹, Mark Ridgeway², Melvin Park², Gary Eiceman³
and Francisco Fernandez-Lima^{1,*}

¹*Department of Chemistry and Biochemistry, Florida International University, Miami,
FL 33199, USA.*

²*Bruker Daltonics, Inc., Billerica, Massachusetts 01821, USA*

³*Department of Chemistry, New Mexico State University, Las Cruces, NM*

Figure S1. Optimized structures of the molecular adduct complexes of TNT, RDX, PETN and HMS.

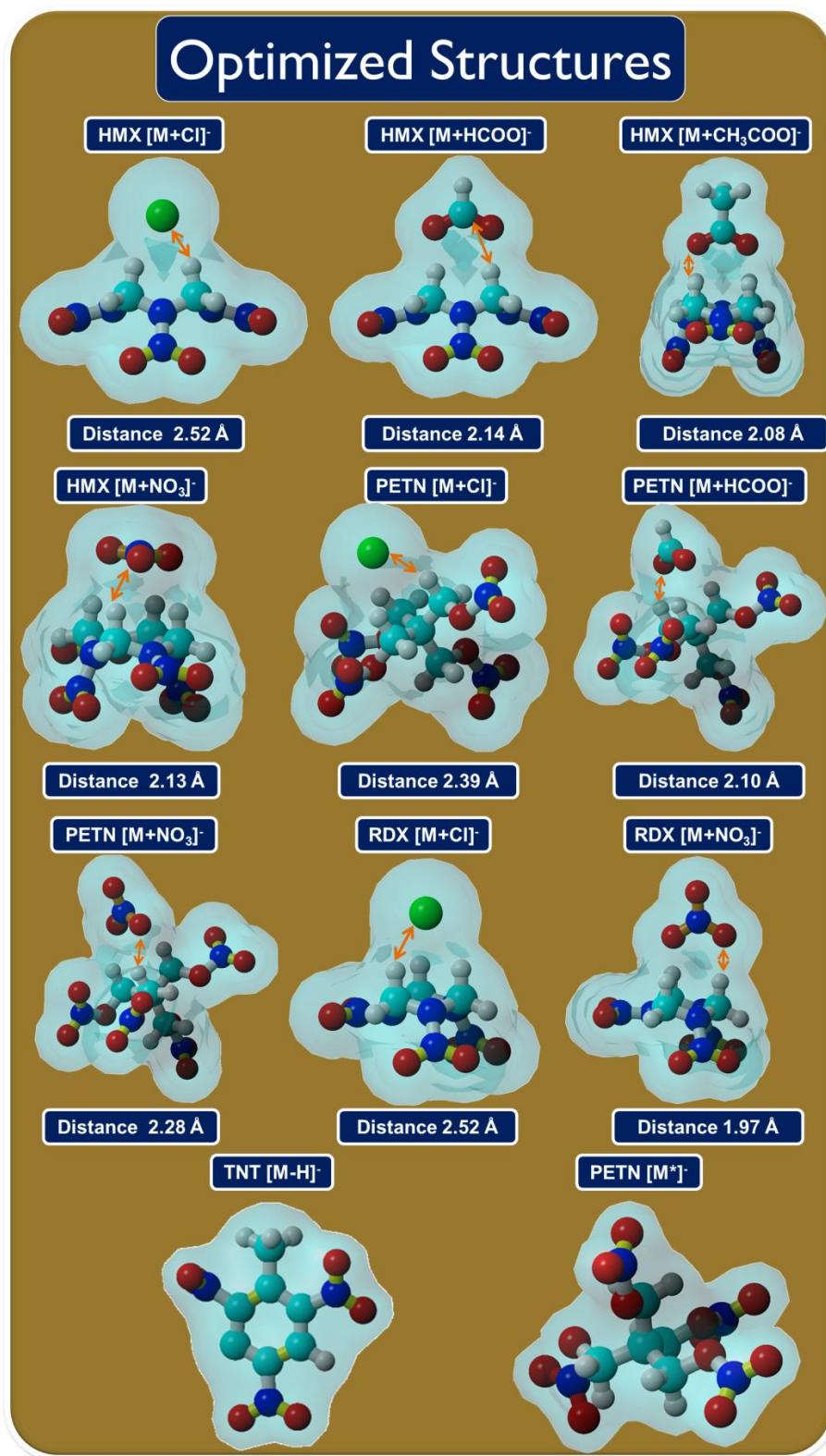
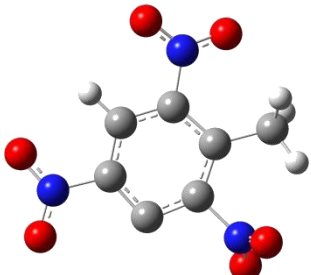
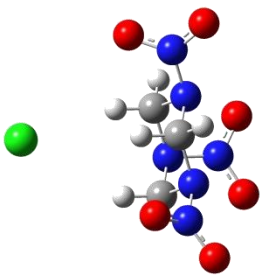


Table S1. Optimized geometry files, charges and structures utilized to calculate the CCS in MOBCAL.

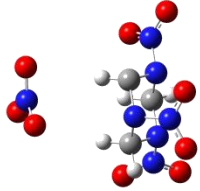
TNT				
[M-H] ⁻				
1				
20				
ang				
calc				
1				
				
X	Y	Z	Atom #	ESP Charges
2.750958	0.001056	0	12	-0.669564
1.403681	0.000544	0	12	0.025134
0.569041	-1.231409	0	12	0.145063
-0.806829	-1.214515	0	12	-0.423731
-1.510661	-0.000584	0	12	0.249954
-0.807779	1.213893	0	12	-0.423704
0.568081	1.231861	0	12	0.145039
1.144085	2.561020	0	14	0.671619
0.400576	3.548814	0	16	-0.514657
2.357861	2.691424	0	16	-0.480116
-2.935022	-0.001138	0	14	0.602739
-3.534707	1.094430	0	16	-0.492816

-3.533853	-1.097178	0	16	-0.492818
1.146090	-2.560135	0	14	0.671627
2.359979	-2.689581	0	16	-0.480112
0.403334	-3.548510	0	16	-0.51466
3.296371	-0.926327	0	1	0.246534
3.295656	0.928867	0	1	0.246533
-1.350450	-2.148101	0	1	0.243972
-1.352119	2.147059	0	1	0.243964

RDX				
[M+Cl] ⁻				
1				
22				
ang				
calc				
1				
				
X	Y	Z	Atom #	ESP Charges
-0.713117	-0.016687	1.243280	12	-0.127403
0.619782	0.566343	1.201934	14	-0.197300
0.910031	1.343218	-0.011003	12	-0.130355
0.617745	0.549083	-1.212368	14	-0.201476

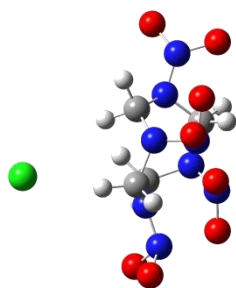
-0.715507	-0.033988	-1.243061	12	-0.127207
-0.899125	-0.811955	0.005695	14	-0.000726
-1.894963	-1.762041	0.013296	14	0.669666
-2.290512	-2.177815	-1.079877	16	-0.446854
-2.287502	-2.163428	1.112897	16	-0.446630
1.660379	-0.176823	-1.800776	14	0.723680
2.804102	0.226112	-1.598055	16	-0.415474
1.353722	-1.110668	-2.542383	16	-0.437511
1.663566	-0.148554	1.801307	14	0.719455
1.358562	-1.072245	2.556241	16	-0.436646
2.806508	0.253817	1.593173	16	-0.414519
-1.422181	0.824994	1.246455	1	0.184649
-0.823003	-0.658809	2.108460	1	0.183495
1.941960	1.673930	-0.014281	1	0.199214
0.195156	2.177577	-0.016474	1	0.179116
-0.827308	-0.687995	-2.099040	1	0.183703
-1.424307	0.807813	-1.256862	1	0.185191
-2.168205	2.879334	-0.017832	28	-0.846069

RDX

[M+NO ₃] ⁻				
1				
25				
ang				
calc				
1				
				
X	Y	Z	Atom #	ESP Charges
0.03258	0.641167	1.242867	12	-0.166948
-0.468995	-0.723678	1.205694	14	-0.220514
-0.115485	-1.477992	-0.005767	12	-0.257471
-0.475011	-0.716824	-1.211301	14	-0.225139
0.025891	0.648492	-1.24324	12	-0.160871
-0.408752	1.324192	0.002945	14	0.013967
-0.381243	2.703634	0.006797	14	0.680895
-0.396326	3.272373	-1.087548	16	-0.444198
-0.39073	3.266147	1.10439	16	-0.444151
-1.725521	-0.95777	-1.80095	14	0.762461
-2.235039	-2.056302	-1.595706	16	-0.417753
-2.178725	-0.087199	-2.543972	16	-0.445293
-1.716304	-0.967894	1.800497	14	0.760397
-2.165514	-0.101447	2.550749	16	-0.444888
-2.22704	-2.065194	1.591677	16	-0.417464
1.127983	0.581989	1.25124	1	0.216803

-0.358221	1.167563	2.105014	1	0.191861
-0.61223	-2.441391	-0.007271	1	0.23686
0.97879	-1.587643	-0.008425	1	0.291573
-0.369972	1.179566	-2.100184	1	0.190476
1.12119	0.589879	-1.258397	1	0.214791
2.997374	-1.786698	0.006186	16	-0.655485
3.608052	-0.67423	-0.004122	14	0.986512
2.922515	0.403481	-0.007499	16	-0.664811
4.852105	-0.629157	-0.011032	16	-0.581608

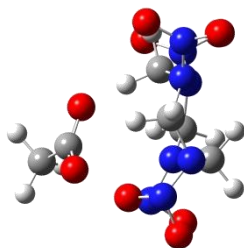
HMX				
[M+Cl] ⁻				
1				
29				
ang				
calc				
1				
X	Y	Z	Atom #	ESP Charges
-1.280590	0.636044	1.265014	12	-0.363223
-0.000016	0.000149	1.537468	14	0.115953
1.280499	0.636218	1.265060	12	-0.360283
1.877347	0.186910	0.000012	14	0.238469
1.280511	0.635944	-1.265129	12	-0.360285



0.000013	-0.000204	-1.537450	14	0.115972
-1.280546	0.635784	-1.265121	12	-0.363187
-1.877342	0.186465	-0.000021	14	0.218278
-3.217196	-0.170829	0.000007	14	0.630980
-3.768397	-0.319063	1.092173	16	-0.439021
-3.768403	-0.319315	-1.092122	16	-0.439017
0.000071	-1.290322	-2.040773	14	0.534527
1.097690	-1.808244	-2.248100	16	-0.392940
-1.097500	-1.808293	-2.248249	16	-0.390763
3.217054	-0.170857	0.000034	14	0.613797
3.768248	-0.319260	1.092185	16	-0.435060
3.768183	-0.319507	-1.092115	16	-0.435060
0.000034	-1.289889	2.041029	14	0.534547
-1.097540	-1.807833	2.248544	16	-0.390762
1.097648	-1.807786	2.248435	16	-0.392943
-1.078510	1.712935	1.194856	1	0.191220
-1.984776	0.411115	2.060108	1	0.205810
1.984700	0.411298	2.060146	1	0.204645
1.078269	1.713093	1.195046	1	0.186312
1.984740	0.410909	-2.060159	1	0.204653
1.078224	1.712816	-1.195306	1	0.186301
-1.984729	0.410784	-2.060198	1	0.205793
-1.078381	1.712665	-1.195110	1	0.191209

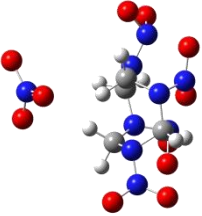
0.000120	3.656170	-0.000380	28	-0.815922
----------	----------	-----------	----	-----------

HMX
[M+CH ₃ COOH-H] ⁻
1
35
ang
calc
1.0000



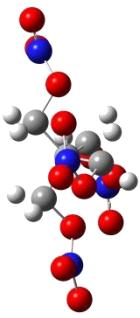
X	Y	Z	Atom #	ESP Charges
-1.256969	0.355496	1.268469	12	-0.595280
-0.036181	-0.398945	1.514136	14	0.359245
1.290653	0.148889	1.268003	12	-0.622339
1.866985	-0.316121	0.000024	14	0.319646
1.290605	0.148486	-1.268061	12	-0.622135
-0.036024	-0.399862	-1.514281	14	0.359092
-1.257100	0.354333	-1.269470	12	-0.595410
-1.901106	-0.010740	-0.000286	14	0.275302
-3.261611	-0.256689	-0.000129	14	0.620637
-3.825917	-0.355017	1.092297	16	-0.436176
-3.825900	-0.356240	-1.092460	16	-0.436190
-0.140597	-1.692730	-1.993879	14	0.462673
0.911628	-2.301906	-2.191492	16	-0.382661

-1.276932	-2.125713	-2.190609	16	-0.381439
3.162585	-0.798420	0.000097	14	0.626215
3.700689	-0.994014	1.092591	16	-0.443151
3.700833	-0.994089	-1.092312	16	-0.443138
-0.141297	-1.691415	1.994645	14	0.462633
-1.277839	-2.123827	2.191457	16	-0.381419
0.910659	-2.300854	2.192906	16	-0.382691
-0.950158	1.410644	1.237537	1	0.300891
-1.974184	0.174274	2.063303	1	0.230014
1.968631	-0.144450	2.063795	1	0.238066
1.156960	1.239550	1.235077	1	0.297998
1.968793	-0.144660	-2.063750	1	0.237992
1.156454	1.239092	-1.235265	1	0.297896
-1.974227	0.171846	-2.064089	1	0.230061
-0.950853	1.409666	-1.239618	1	0.300954
1.556955	5.446514	-0.004656	1	0.091316
0.483040	5.214906	-0.001065	12	-0.442257
0.307047	3.688081	-0.000230	12	0.975277
0.047361	5.659254	0.899601	1	0.086128
0.041712	5.658747	-0.899246	1	0.086167
0.255940	3.112050	1.127833	16	-0.846886
0.254290	3.111214	-1.127817	16	-0.847029

HMX				
[M+NO ₃] ⁻				
1				
32				
ang				
calc				
1				
				
X	Y	Z	Atom #	ESP Charges
1.285739	0.376327	-1.280849	12	-0.189881
0.026455	-0.309189	-1.531470	14	-0.142322
-1.284264	0.273035	-1.280705	12	0.014395
-1.863430	-0.157011	-0.003823	14	0.099583
-1.285166	0.311965	1.259884	12	-0.167862
0.024492	-0.267296	1.526700	14	0.113122
1.283734	0.414019	1.261350	12	-0.234359
1.898518	-0.005706	-0.003416	14	0.128115
3.251579	-0.320952	0.001941	14	0.624758
3.805773	-0.470362	-1.087443	16	-0.428573
3.806053	-0.431718	1.095731	16	-0.429318
0.075098	-1.559268	2.026318	14	0.483787
-1.001112	-2.120401	2.230874	16	-0.380974
1.191909	-2.035061	2.229832	16	-0.374731
-3.185182	-0.586281	0.001982	14	0.620406

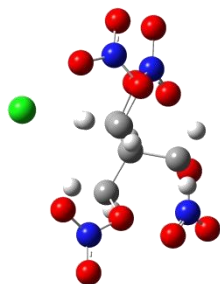
-3.724412	-0.783096	-1.087124	16	-0.427641
-3.727641	-0.743298	1.095869	16	-0.428025
0.078332	-1.614322	-1.998882	14	0.618244
1.195457	-2.094285	-2.188781	16	-0.399743
-0.997205	-2.180394	-2.191518	16	-0.410982
1.074972	1.452926	-1.279446	1	0.159732
1.997346	0.135570	-2.065084	1	0.193332
-1.973640	-0.024363	-2.065317	1	0.143560
-1.166197	1.362599	-1.278004	1	0.067653
-1.975172	0.039033	2.052765	1	0.171936
-1.150499	1.398906	1.236171	1	0.089801
1.993502	0.195795	2.053793	1	0.188121
1.060787	1.487698	1.238804	1	0.122826
0.788575	3.512218	-0.793544	16	-0.590839
-0.207442	3.446332	-0.019958	14	0.909188
-1.376827	3.397796	-0.491810	16	-0.573864
-0.029357	3.363054	1.231976	16	-0.569446



PETN				
[M*]				
1				
29				
ang				
calc				
1				
				
X	Y	Z	Atom #	ESP Charges
0.687075	-1.248249	0.170054	12	0.064415
-0.181022	-0.125539	-0.440166	12	-0.189551
-1.435950	-0.792734	-1.052582	12	-0.074121
-2.145811	-1.427387	0.031183	16	-0.314517
-3.374501	-2.049077	-0.361118	14	0.845912
-3.950403	-2.553061	0.567730	16	-0.365996
-3.668258	-1.995465	-1.536456	16	-0.384242
0.507790	0.589464	-1.632509	12	0.136217
1.610596	1.421791	-1.235376	16	-0.312479
2.919887	0.852080	-1.396063	14	0.724347
3.781643	1.592832	-1.007776	16	-0.312007
3.001803	-0.250498	-1.897271	16	-0.348838
-0.557918	0.881428	0.666742	12	0.387326
-1.489633	1.806863	0.060723	16	-0.357593
-1.921452	2.855443	0.927776	14	0.811406

-1.487957	2.850645	2.059604	16	-0.381509
-2.684053	3.615239	0.385767	16	-0.364884
1.795080	-0.618961	0.848584	16	-0.337221
2.671790	-1.546475	1.502612	14	0.814449
2.393732	-2.723260	1.412155	16	-0.385258
3.584383	-0.998185	2.062901	16	-0.345229
1.066114	-1.910439	-0.614123	1	0.118227
0.111027	-1.835572	0.888696	1	0.104091
-1.155424	-1.546327	-1.796025	1	0.128234
-2.080691	-0.048046	-1.523387	1	0.129816
-0.186791	1.295998	-2.093514	1	0.080991
0.841553	-0.129568	-2.383565	1	0.083990
0.322778	1.421210	1.016318	1	0.018640
-1.037457	0.378303	1.509769	1	0.025383

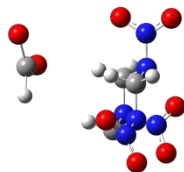
PETN
[M+Cl] ⁻
1
30
ang
calc
1



X	Y	Z	Atom #	ESP Charges
0.563563	-0.964377	0.785729	12	0.172219
-0.230054	-0.051086	-0.172515	12	-0.392951
-1.492050	-0.826356	-0.616348	12	0.311580
-2.266007	-1.069333	0.598339	16	-0.366140
-3.535056	-1.624931	0.385449	14	0.864343
-4.121839	-1.868897	1.419947	16	-0.427488
-3.906332	-1.781471	-0.760358	16	-0.420999
0.562017	0.220982	-1.483053	12	0.118964
1.464270	1.345506	-1.324947	16	-0.286649
2.858137	1.057520	-1.315189	14	0.707488
3.518608	2.056076	-1.126194	16	-0.381517
3.218937	-0.079854	-1.504283	16	-0.320947
-0.595159	1.252701	0.562524	12	0.172809
-1.416057	2.030201	-0.354582	16	-0.294759
-1.800732	3.288415	0.129742	14	0.827592
-1.447446	3.599680	1.252065	16	-0.407256
-2.464444	3.919721	-0.663366	16	-0.411283
1.728107	-0.195539	1.215128	16	-0.274024
2.539755	-0.844984	2.160320	14	0.815431
2.174944	-1.926713	2.575658	16	-0.410372
3.524669	-0.202754	2.456536	16	-0.410883
0.877109	-1.869299	0.249864	1	0.146215

-0.025319	-1.227270	1.666943	1	0.055739
-1.204415	-1.780358	-1.081224	1	0.071452
-2.094796	-0.225216	-1.299313	1	0.042369
-0.113781	0.543075	-2.279205	1	0.073036
1.085006	-0.684568	-1.806701	1	0.136377
0.294223	1.828440	0.815440	1	0.068963
-1.174180	1.045607	1.465375	1	0.076086
0.530132	-3.245101	-1.881353	28	-0.855393

PETN
[M+HCOOH-H] ⁻
1
33
ang
calc
1

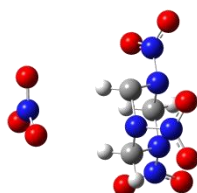


X	Y	Z	Atom #	ESP Charges
0.664108	-0.588581	0.972726	12	0.291904
-0.206842	0.050524	-0.130732	12	-0.401483
-1.369220	-0.936344	-0.396658	12	0.096443
-2.193972	-0.915612	0.811006	16	-0.344014
-3.357466	-1.690244	0.739094	14	0.853621
-3.984227	-1.697971	1.779606	16	-0.427554

-3.617716	-2.236721	-0.313812	16	-0.415266
0.534647	0.173225	-1.487125	12	0.089189
1.484868	1.272570	-1.491141	16	-0.351482
2.854499	0.932257	-1.355837	14	0.771120
3.569821	1.910386	-1.398844	16	-0.393132
3.155079	-0.232674	-1.228236	16	-0.370137
-0.708639	1.421997	0.363057	12	0.375098
-1.654866	1.903445	-0.633824	16	-0.327763
-2.200040	3.164427	-0.358524	14	0.831139
-1.858876	3.722333	0.668210	16	-0.423907
-2.972324	3.544918	-1.211585	16	-0.408788
1.697529	0.385697	1.315632	16	-0.362068
2.528479	0.002800	2.379839	14	0.800723
2.291135	-1.049876	2.938311	16	-0.415011
3.398841	0.814355	2.615317	16	-0.396090
1.104283	-1.522771	0.609636	1	0.181328
0.071242	-0.789112	1.868048	1	0.035447
-0.970770	-1.944845	-0.556520	1	0.213281
-1.979029	-0.613243	-1.241677	1	0.078308
-0.169042	0.467979	-2.269241	1	0.084733
0.988983	-0.779349	-1.784108	1	0.254448
0.111264	2.135281	0.444892	1	0.039880
-1.222370	1.335301	1.322423	1	0.017252

0.661092	-2.716344	-2.530845	16	-0.857534
0.764845	-3.577729	-1.618348	12	0.860255
0.538648	-3.430969	-0.383045	16	-0.861746
1.093485	-4.600771	-1.936973	1	-0.118194

PETN
[M+NO ₃] ⁻
1
33
ang
calc
1



X	Y	Z	Atom #	ESP Charges
-0.668410	-0.031337	1.100097	12	0.349655
0.312602	-0.124288	-0.089343	12	-0.370339
0.981876	1.264550	-0.227630	12	0.160322
1.800541	1.432355	0.969724	16	-0.349897
2.577494	2.601769	0.988934	14	0.839424
3.201815	2.733377	2.020997	16	-0.417886
2.554808	3.317286	0.008879	16	-0.401504
-0.410052	-0.364075	-1.440397	12	0.089751
-0.832182	-1.742946	-1.597890	16	-0.350964
-2.212039	-2.013698	-1.391847	14	0.756401

-2.469904	-3.185986	-1.550353	16	-0.375241
-2.947245	-1.095522	-1.107405	16	-0.361948
1.343325	-1.233172	0.202695	12	0.293716
2.332199	-1.171249	-0.863062	16	-0.330996
3.347876	-2.135970	-0.771987	14	0.845417
3.323576	-2.900176	0.174558	16	-0.422432
4.144863	-2.071977	-1.681716	16	-0.408770
-1.196860	-1.373528	1.317423	16	-0.379422
-2.047991	-1.491460	2.432869	14	0.800579
-2.225792	-0.504544	3.117616	16	-0.406767
-2.494478	-2.609906	2.566872	16	-0.388113
-1.474911	0.671078	0.872911	1	0.136316
-0.151054	0.288372	2.007340	1	0.023753
0.221431	2.049462	-0.271427	1	0.162130
1.629607	1.303703	-1.104596	1	0.065497
0.290394	-0.231052	-2.268105	1	0.101815
-1.238335	0.335091	-1.576071	1	0.212662
0.876665	-2.217907	0.195413	1	0.059118
1.842993	-1.067094	1.159114	1	0.035136
-1.771549	2.829599	0.159662	16	-0.715352
-2.091940	3.121052	-1.039526	14	1.075163
-2.896864	4.041792	-1.274740	16	-0.598235
-1.568758	2.454728	-1.987593	16	-0.728987

