Supplementary Information

Title: Arginine zwitterion is more stable than canonical form when Solvated by a water molecule

Authors: Suk Im, Sung-Woo Jang, Sungyul Lee, Yonghoon Lee, Bongsoo Kim

Supplementary Table 1 Energy (Hartree), ZPE (kcal/mol) and Gibbs function (kcal/mol) for the structures of zwitterionic Arg - H_2O depicted in Fig. 1 and Fig. 3 (B3LPY/6-311++G**)

(Z22-1)

	E	ZPE	G(5 °K)
	-683.22550	156.31889	-428418.0145

Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.289174	-0.413198	-1.192335
2	6	0	1.955987	-0.842625	0.186192
3	6	0	0.540076	-1.489064	0.154224
4	8	0	0.208721	-2.001394	-0.948077
5	6	0	2.130773	0.317483	1.185596
6	6	0	1.052888	1.416809	1.259148
7	6	0	0.684120	2.128151	-0.052090
8	7	0	-0.046655	1.280346	-1.004706

9	6	0	-1.302245	0.862780	-0.828554
10	7	0	-1.751668	-0.204826	-1.504589
11	7	0	-2.165537	1.523854	-0.019773
12	8	0	-0.157322	-1.416615	1.196012
13	1	0	2.063580	-1.186367	-1.814054
14	1	0	0.586203	0.668606	-1.532607
15	1	0	-1.068727	-0.981141	-1.590992
16	1	0	-2.662525	-0.530545	-1.205859
17	1	0	-2.797442	0.906424	0.491090
18	1	0	-1.798965	2.289291	0.522300
19	1	0	2.632453	-1.645231	0.517990
20	1	0	2.204792	-0.115947	2.186098
21	1	0	3.104823	0.783057	0.982163
22	1	0	0.152426	0.986397	1.702984
23	1	0	1.411590	2.187101	1.952236
24	1	0	0.098997	3.030173	0.151613
25	1	0	1.579539	2.463349	-0.578730
26	1	0	3.281586	-0.214434	-1.277605
27	1	0	-3.329107	-1.598792	1.720227
28	8	0	-2.829704	-1.007376	1.151620
29	1	0	-1.879571	-1.303288	1.199422

(Z21-2)

	E	ZPE	G(5 °K)
	-683.22471	156.39231	-428417.3746

Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.167493	-0.661503	1.258871

2	6	0	-1.906479	-0.968836	-0.164183
3	6	0	-0.426083	-1.450801	-0.269275
4	8	0	0.001610	-2.063584	0.746701
5	6	0	-2.275237	0.218003	-1.074396
6	6	0	-1.976829	1.632987	-0.543453
7	6	0	-0.504006	1.990107	-0.325158
8	7	0	0.080327	1.231063	0.792130
9	6	0	1.360702	0.865571	0.828757
10	7	0	2.306096	1.536862	0.126623
11	7	0	1.740776	-0.167710	1.596166
12	8	0	0.214534	-1.181664	-1.313923
13	1	0	-1.820049	-1.444733	1.806934
14	1	0	-0.592774	0.681750	1.343149
15	1	0	1.993887	2.320275	-0.426018
16	1	0	2.958541	0.918798	-0.360629
17	1	0	2.722809	-0.396972	1.533011
18	1	0	1.116259	-0.997507	1.540875
19	1	0	-2.500460	-1.830991	-0.504605
20	1	0	-1.769476	0.063493	-2.030491
21	1	0	-3.352370	0.179599	-1.276097
22	1	0	-2.363031	2.352719	-1.272809
23	1	0	-2.527325	1.816146	0.384510
24	1	0	0.059086	1.763022	-1.235477
25	1	0	-0.421365	3.063813	-0.120799
26	1	0	-3.162213	-0.560308	1.438731
27	1	0	1.946443	-1.097151	-1.341740
28	8	0	2.903311	-0.827952	-1.296363
29	1	0	3.406052	-1.539533	-1.700131

Supplementary Table 2 Energy (Hartree), ZPE (kcal/mol) and Gibbs function (kcal/mol) for the structures of canonical Arg - H_2O depicted in Fig. 2 and Fig. 3 (B3LPY/6-311++G**)

(C4-1)

	E	ZPE	G(5 °K)
	-683.21962	154.58195	-428417.8015

Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.743302	-1.699184	-0.164235
2	6	0	-0.601869	-1.883748	-1.178011
3	6	0	0.819970	-1.864985	-0.599481
4	7	0	1.232318	-0.509507	-0.242767
5	6	0	2.403632	-0.304483	0.266906
6	7	0	2.794877	0.947211	0.667177
7	6	0	-1.782743	-0.405361	0.683091
8	6	0	-1.821718	0.859695	-0.203084
9	8	0	-2.836641	1.480748	-0.410419
10	7	0	-2.916927	-0.491761	1.599035
11	8	0	-0.647347	1.238142	-0.729062
12	7	0	3.351885	-1.295069	0.453815
13	1	0	-3.778789	-0.356504	1.076183
14	1	0	0.120524	0.576488	-0.513685
15	1	0	3.027195	-2.247876	0.411430
16	1	0	4.041549	-1.133811	1.172350
17	1	0	3.787085	1.128600	0.672713
18	1	0	2.233595	1.739978	0.354392
19	1	0	-0.871692	-0.355927	1.285691
20	1	0	-1.729801	-2.525697	0.553150

21	1	0	-2.697062	-1.774205	-0.699775
22	1	0	-0.751441	-2.856009	-1.659070
23	1	0	-0.663576	-1.138591	-1.977171
24	1	0	0.855489	-2.537626	0.274648
25	1	0	1.501061	-2.283959	-1.354488
26	1	0	-2.881523	0.270933	2.268585
27	1	0	0.332598	2.823527	-0.498289
28	8	0	1.147581	3.268525	-0.202154
29	1	0	1.287163	4.003638	-0.805516

(C4-7)

	E	ZPE	G(5 °K)
	-683.21968	154.54680	-428417.9089

Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.747215	-1.699654	-0.175697
2	6	0	-0.596021	-1.887657	-1.177786
3	6	0	0.820399	-1.870168	-0.585761
4	7	0	1.227820	-0.514673	-0.223434
5	6	0	2.400747	-0.303661	0.279023
6	7	0	2.784781	0.949609	0.687547
7	6	0	-1.789594	-0.409172	0.677017
8	6	0	-1.818045	0.863622	-0.199054
9	8	0	-2.824999	1.505110	-0.385525
10	7	0	-2.929107	-0.498978	1.586119
11	8	0	-0.645582	1.225801	-0.736450
12	7	0	3.358804	-1.286016	0.451878

13	1	0	-3.788272	-0.366223	1.058223
14	1	0	0.120570	0.563974	-0.512023
15	1	0	3.047391	-2.242372	0.395555
16	1	0	4.052716	-1.124467	1.166069
17	1	0	3.774021	1.145025	0.643614
18	1	0	2.207119	1.734119	0.383711
19	1	0	-0.881873	-0.366156	1.285434
20	1	0	-1.745445	-2.528399	0.539166
21	1	0	-2.695504	-1.768658	-0.721712
22	1	0	-0.742693	-2.860379	-1.658735
23	1	0	-0.648471	-1.143685	-1.978535
24	1	0	0.849765	-2.543545	0.287833
25	1	0	1.507803	-2.287097	-1.336111
26	1	0	-2.900738	0.264464	2.255126
27	1	0	0.367216	2.817751	-0.599077
28	8	0	1.197082	3.254927	-0.335112
29	1	0	0.946680	4.109485	0.026926

(C5-1)

	E	ZPE	G(5 °K)
	-683.21998	154.53865	-428418.1193

Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.787623	-1.673377	-0.221287
2	6	0	-0.609347	-1.870010	-1.189893
3	6	0	0.784947	-1.881171	-0.546135
4	7	0	1.228736	-0.527203	-0.218605

5	6	0	2.418474	-0.333283	0.252253
6	7	0	2.932285	0.928875	0.399046
7	6	0	-1.815142	-0.404190	0.662559
8	6	0	-1.813109	0.885667	-0.186670
9	8	0	-2.812412	1.531752	-0.393964
10	7	0	-2.966401	-0.492738	1.557121
11	8	0	-0.623125	1.256182	-0.680329
12	7	0	3.276687	-1.344656	0.643473
13	1	0	-3.816364	-0.329380	1.022873
14	1	0	0.131328	0.575714	-0.472260
15	1	0	4.264801	-1.156365	0.568099
16	1	0	3.016290	-2.288004	0.406446
17	1	0	2.325561	1.721848	0.188875
18	1	0	3.561789	1.075477	1.173547
19	1	0	-0.913415	-0.392781	1.281433
20	1	0	-1.830343	-2.518507	0.472655
21	1	0	-2.720431	-1.701264	-0.796625
22	1	0	-0.757627	-2.835096	-1.685259
23	1	0	-0.621683	-1.116630	-1.983484
24	1	0	0.753614	-2.519347	0.351665
25	1	0	1.486678	-2.352017	-1.251458
26	1	0	-2.929856	0.253842	2.244597
27	1	0	0.362774	2.829341	-0.414452
28	8	0	1.185145	3.270005	-0.132389
29	1	0	1.321669	3.997895	-0.745400

Supplementary Table 3 Energy (Hartree), ZPE (kcal/mol) and Gibbs function (kcal/mol) for the structures of zwitterionic Arg -H_2O depicted in Fig. 1 (MP2/aug-cc-pvdz)

(Z22-1)

	E	ZPE	G(5 °K)
	-681.26117	156.55044	-427184.9161

Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.341619	-0.532834	-1.095180
2	6	0	1.914045	-0.885579	0.282755
3	6	0	0.468218	-1.434154	0.201390
4	8	0	0.167391	-2.013600	-0.893666
5	6	0	2.100640	0.310075	1.235788
6	6	0	1.072571	1.455943	1.179419
7	6	0	0.800303	2.041075	-0.214456
8	7	0	0.035775	1.133986	-1.079536
9	6	0	-1.241687	0.807943	-0.850689
10	7	0	-1.779247	-0.263355	-1.465866
11	7	0	-2.041741	1.588989	-0.072498
12	8	0	-0.288531	-1.242449	1.203495
13	1	0	2.145360	-1.347935	-1.682317
14	1	0	0.628430	0.443687	-1.560902
15	1	0	-1.124620	-1.077027	-1.505151
16	1	0	-2.696841	-0.516237	-1.104795
17	1	0	-2.719656	1.043544	0.467890
18	1	0	-1.581836	2.321075	0.454137
19	1	0	2.523766	-1.718865	0.687472
20	1	0	2.099527	-0.077825	2.267125
21	1	0	3.112308	0.722054	1.055242

22	1	0	0.127757	1.098321	1.617551
23	1	0	1.443294	2.277909	1.818370
24	1	0	0.267160	3.004808	-0.144497
25	1	0	1.740551	2.242418	-0.748626
26	1	0	3.351640	-0.379365	-1.114925
27	1	0	-3.411524	-1.375014	1.780656
28	8	0	-2.940902	-0.841859	1.129607
29	1	0	-1.988353	-1.137602	1.183598

(Z21-2)

	E	ZPE	G(5 °K)
	-681.26007	156.46698	-427184.3902

Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.088115	-0.781526	1.252676
2	6	0	-1.852977	-1.022998	-0.193725
3	6	0	-0.349028	-1.381571	-0.343403
4	8	0	0.114661	-2.093238	0.607720
5	6	0	-2.334820	0.169971	-1.034859
6	6	0	-2.073266	1.568704	-0.446174
7	6	0	-0.596719	1.932802	-0.274859
8	7	0	0.004361	1.158328	0.821976
9	6	0	1.304659	0.852390	0.820350
10	7	0	2.201369	1.614263	0.135123
11	7	0	1.756568	-0.187637	1.551477
12	8	0	0.287216	-0.943495	-1.351652
13	1	0	-1.731096	-1.602645	1.748111
14	1	0	-0.645079	0.532684	1.335986

15	1	0	1.815485	2.372554	-0.415017
16	1	0	2.898747	1.050269	-0.361140
17	1	0	2.745594	-0.375173	1.410552
18	1	0	1.163595	-1.041658	1.444114
19	1	0	-2.395560	-1.922458	-0.548264
20	1	0	-1.862437	0.088474	-2.027022
21	1	0	-3.425850	0.076622	-1.183859
22	1	0	-2.508438	2.315285	-1.132333
23	1	0	-2.591250	1.690535	0.520126
24	1	0	-0.057754	1.693700	-1.208179
25	1	0	-0.502075	3.012163	-0.061647
26	1	0	-3.089851	-0.715613	1.445323
27	1	0	2.008044	-0.955141	-1.282175
28	8	0	2.977097	-0.733729	-1.188818
29	1	0	3.439755	-1.395693	-1.715307

Supplementary Table 4 Energy (Hartree), ZPE (kcal/mol) and Gibbs function (kcal/mol) for the structures of canonical Arg - H_2O depicted in Fig. 2 (MP2/aug-cc-pvdz)

(C4-1)

	E	ZPE	G(5 °K)
	-681.24993	154.79718	-427181.3763

Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.666717	-1.727680	-0.075765
2	6	0	-0.590599	-1.908496	-1.159693
3	6	0	0.848366	-1.847660	-0.630903
4	7	0	1.218097	-0.463889	-0.311408
5	6	0	2.379370	-0.244226	0.238974
6	7	0	2.741311	1.017724	0.665005
7	6	0	-1.659328	-0.402461	0.717359
8	6	0	-1.829838	0.787856	-0.241802
9	8	0	-2.910780	1.325122	-0.440719
10	7	0	-2.717632	-0.473928	1.729322
11	8	0	-0.706905	1.199869	-0.876098
12	7	0	3.345537	-1.222174	0.451002
13	1	0	-3.615379	-0.365494	1.248325
14	1	0	0.087873	0.583372	-0.628815
15	1	0	3.019095	-2.180627	0.399836
16	1	0	3.958257	-1.055100	1.242978
17	1	0	3.733701	1.220892	0.606080
18	1	0	2.149932	1.788541	0.339106
19	1	0	-0.694203	-0.296447	1.238324

20	1	0	-1.576020	-2.535388	0.670848
21	1	0	-2.666271	-1.829456	-0.536823
22	1	0	-0.742462	-2.899911	-1.619822
23	1	0	-0.706927	-1.165129	-1.966141
24	1	0	0.925522	-2.498608	0.266508
25	1	0	1.533942	-2.256078	-1.398718
26	1	0	-2.653593	0.347517	2.334135
27	1	0	0.214183	2.792154	-0.517853
28	8	0	0.984891	3.270593	-0.154925
29	1	0	1.095989	4.036966	-0.730495

(C4-7)

	E	ZPE	G(5 °K)
	-681.24990	154.75388	-427181.4418

Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.690804	-1.712404	-0.119209
2	6	0	-0.599158	-1.885268	-1.188899
3	6	0	0.831991	-1.846738	-0.636984
4	7	0	1.208067	-0.471033	-0.290927
5	6	0	2.370202	-0.265583	0.262405
6	7	0	2.738722	0.988670	0.709623
7	6	0	-1.676290	-0.407981	0.707828
8	6	0	-1.823383	0.812747	-0.217035
9	8	0	-2.891084	1.386482	-0.386868
10	7	0	-2.743243	-0.495671	1.709818
11	8	0	-0.697686	1.208860	-0.852724

12	7	0	3.331819	-1.250470	0.457261
13	1	0	-3.636469	-0.370709	1.224396
14	1	0	0.090461	0.582239	-0.605815
15	1	0	3.004655	-2.207370	0.387424
16	1	0	3.949734	-1.098069	1.247957
17	1	0	3.729924	1.191315	0.625444
18	1	0	2.147487	1.763361	0.392307
19	1	0	-0.714256	-0.328220	1.239430
20	1	0	-1.624785	-2.538848	0.609220
21	1	0	-2.683853	-1.788304	-0.599002
22	1	0	-0.753212	-2.867405	-1.667750
23	1	0	-0.695209	-1.127534	-1.984332
24	1	0	0.891179	-2.511599	0.251432
25	1	0	1.525139	-2.248589	-1.401364
26	1	0	-2.680152	0.312518	2.332336
27	1	0	0.284274	2.799312	-0.593583
28	8	0	1.105042	3.252062	-0.318855
29	1	0	0.812007	4.089578	0.060424

(C5-1)

	E	ZPE	G(5 °K)
	-681.25012	154.81538	-427181.456

Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.712456	-1.710171	-0.119201
2	6	0	-0.594106	-1.908641	-1.156512
3	6	0	0.819800	-1.866824	-0.560831

4	7	0	1.215554	-0.479996	-0.285282
5	6	0	2.398004	-0.263388	0.219925
6	7	0	2.891249	1.016631	0.371997
7	6	0	-1.692224	-0.400113	0.697659
8	6	0	-1.822639	0.810966	-0.241359
9	8	0	-2.888879	1.375333	-0.444710
10	7	0	-2.768217	-0.467461	1.691589
11	8	0	-0.682782	1.210235	-0.851851
12	7	0	3.264807	-1.263296	0.647301
13	1	0	-3.655953	-0.339354	1.196996
14	1	0	0.099827	0.577252	-0.602612
15	1	0	4.250985	-1.035117	0.574120
16	1	0	3.049021	-2.201701	0.330929
17	1	0	2.229846	1.780178	0.198807
18	1	0	3.470719	1.157669	1.193110
19	1	0	-0.733565	-0.324757	1.236405
20	1	0	-1.678025	-2.531430	0.617085
21	1	0	-2.694046	-1.772753	-0.623656
22	1	0	-0.742175	-2.898362	-1.621208
23	1	0	-0.661801	-1.164326	-1.967620
24	1	0	0.835156	-2.476127	0.366531
25	1	0	1.529027	-2.328803	-1.276905
26	1	0	-2.702360	0.346553	2.306278
27	1	0	0.231851	2.789767	-0.434561
28	8	0	1.002756	3.261729	-0.063066
29	1	0	1.120710	4.030801	-0.634011

Supplementary Table 5 Energy (Hartree), ZPE (kcal/mol) and Gibbs function (kcal/mol) for the structures of zwitterionic Arg-H_2O depicted in Fig. 4 (B3LPY/6-311++G**)

(C22-1)

	E	ZPE	G(5 °K)
	-683.21365	155.74535	-428411.7291

Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.018124	-0.584320	1.449335
2	6	0	-1.940816	-0.850099	0.003929
3	6	0	-0.587948	-1.539329	-0.246754
4	8	0	-0.126039	-2.184938	0.825368
5	6	0	-2.274875	0.309775	-0.963700
6	6	0	-1.233301	1.408027	-1.240334
7	6	0	-0.713283	2.209255	-0.029549
8	7	0	0.044714	1.401873	0.917405
9	6	0	1.281605	1.136712	0.656257
10	7	0	2.036239	0.393793	1.550993
11	7	0	2.004733	1.590615	-0.432552
12	8	0	0.004680	-1.552918	-1.305566
13	1	0	-0.746747	-1.922526	1.552074
14	1	0	-1.448933	0.240990	1.668205
15	1	0	1.470677	-0.000089	2.288730
16	1	0	2.636727	-0.294884	1.108966
17	1	0	2.809841	1.028360	-0.677140
18	1	0	1.465065	1.856646	-1.240108
19	1	0	-2.676829	-1.639609	-0.200696

20	1	0	-2.533857	-0.138790	-1.928161
21	1	0	-3.197464	0.767253	-0.585530
22	1	0	-0.395760	0.954040	-1.776963
23	1	0	-1.696976	2.116016	-1.938027
24	1	0	-0.133266	3.068954	-0.398134
25	1	0	-1.568134	2.637656	0.506051
26	1	0	-2.973379	-0.453171	1.759740
27	1	0	3.393723	-2.069673	-1.163285
28	8	0	2.869988	-1.296676	-0.934278
29	1	0	1.945062	-1.534695	-1.135286

Supplementary Table 6 Energy (Hartree), ZPE (kcal/mol) and Gibbs function (kcal/mol) for the structures of zwitterionic Arg-H_2O depicted in Fig. 4 (MP2/6-311+G*)

(C22-1)

	E	ZPE	G(5 °K)
	-681.22489	159.09499	-427157.0606

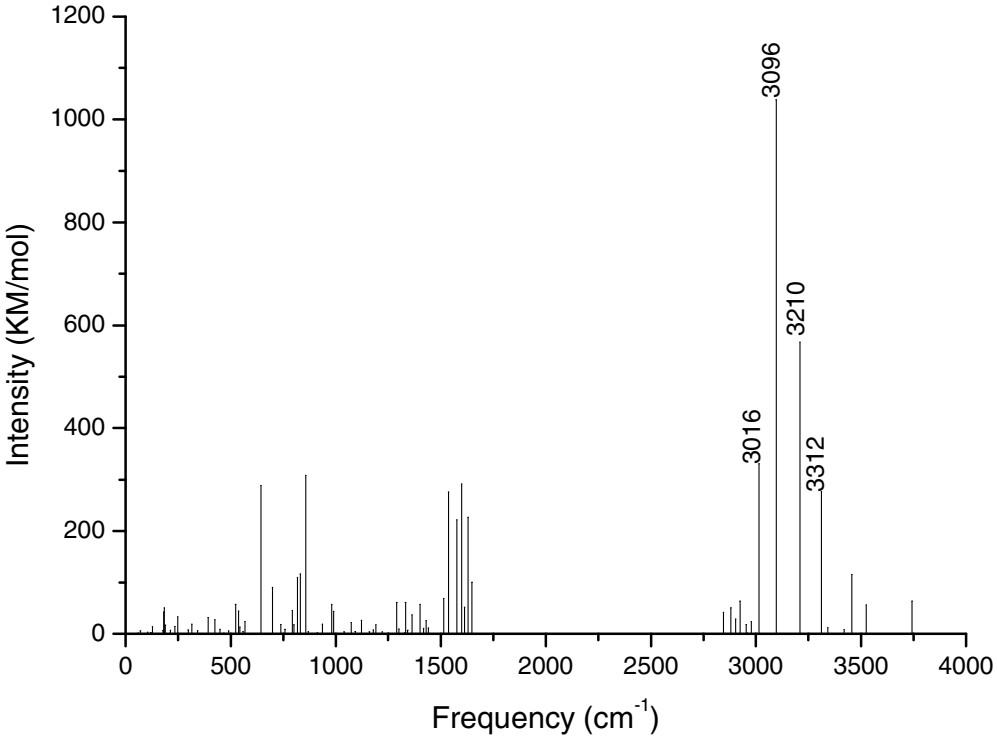
Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.080907	-0.783920	1.360176
2	6	0	-1.890274	-0.933047	-0.087133
3	6	0	-0.464684	-1.448097	-0.302823
4	8	0	0.025447	-2.106179	0.749840
5	6	0	-2.277268	0.248116	-0.996273
6	6	0	-1.288425	1.405441	-1.176941
7	6	0	-0.839902	2.110485	0.109157
8	7	0	-0.072522	1.233400	0.984869
9	6	0	1.183970	1.071237	0.703698
10	7	0	1.989324	0.312819	1.538658
11	7	0	1.878199	1.676510	-0.331120
12	8	0	0.158295	-1.343472	-1.344990
13	1	0	-0.653336	-1.983280	1.455782
14	1	0	-1.610361	0.067173	1.672753
15	1	0	1.438429	-0.176375	2.229080
16	1	0	2.610752	-0.310111	1.032995
17	1	0	2.727637	1.190849	-0.589597
18	1	0	1.325036	1.915440	-1.138400

19	1	0	-2.526155	-1.780337	-0.386706
20	1	0	-2.488096	-0.160290	-1.991969
21	1	0	-3.233358	0.634317	-0.617565
22	1	0	-0.422678	1.025262	-1.726256
23	1	0	-1.772554	2.144743	-1.829305
24	1	0	-0.282556	3.026021	-0.142862
25	1	0	-1.726577	2.440941	0.664194
26	1	0	-3.062978	-0.764835	1.606696
27	1	0	3.617045	-1.695659	-1.272751
28	8	0	2.993930	-1.053992	-0.925160
29	1	0	2.099209	-1.341188	-1.169808

Supplementary Figure 1. Infrared spectra of Arg – (H_2O) conformers (scaling factor = 0.9613) depicted in Fig. 1 and Fig. 2

(Z22-1)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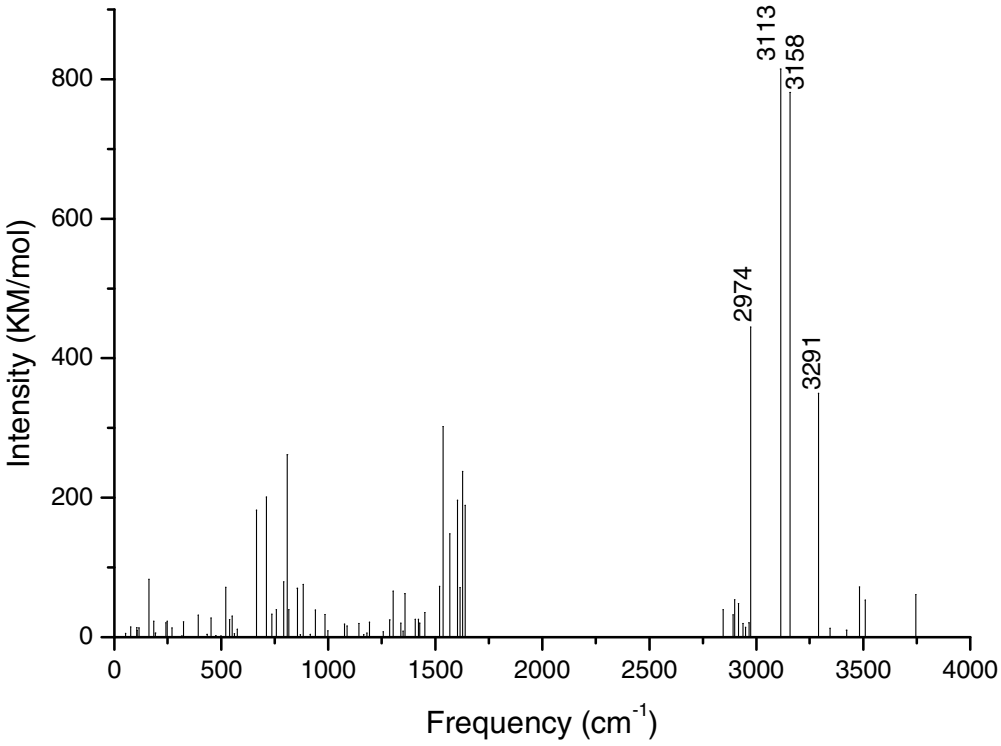
(Z21-2)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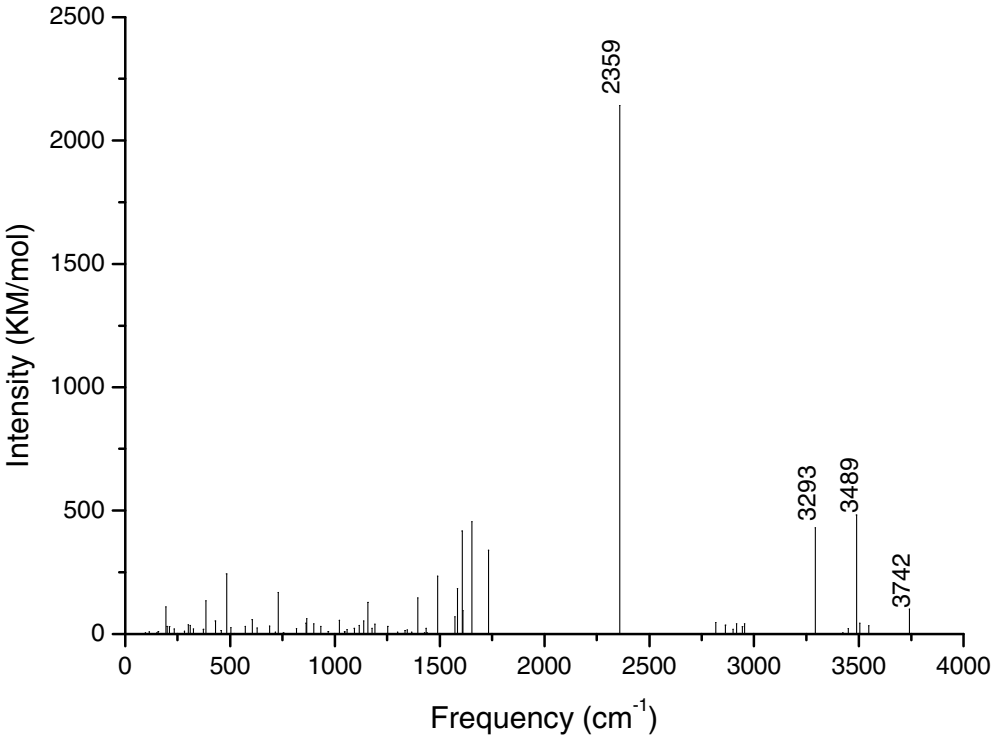
(C4-1)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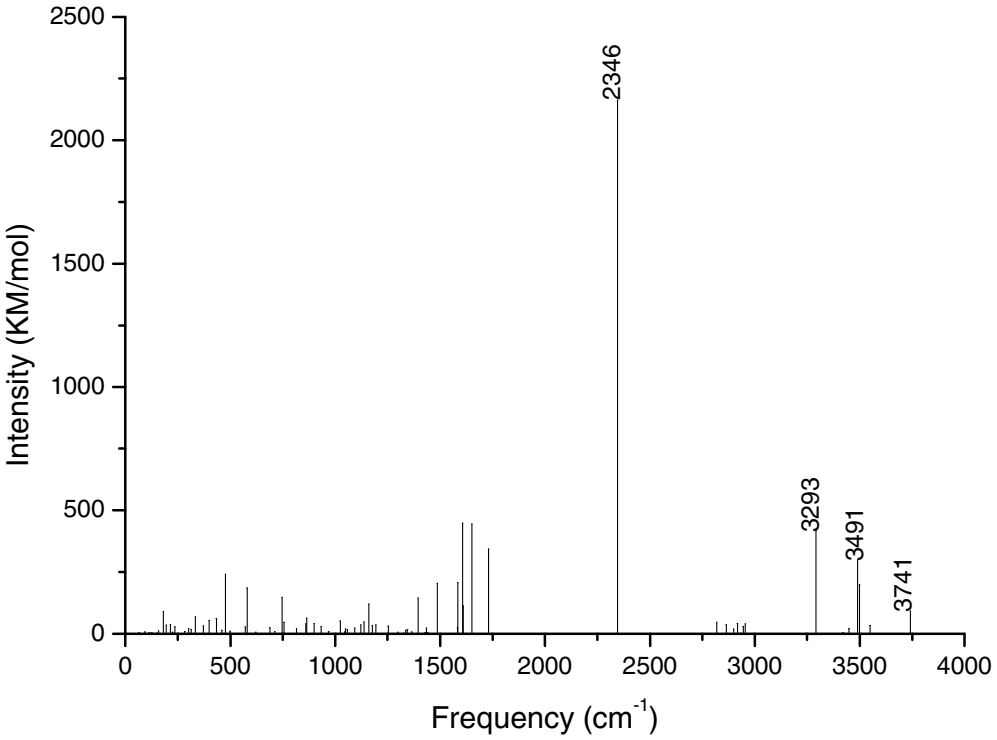
(C4-7)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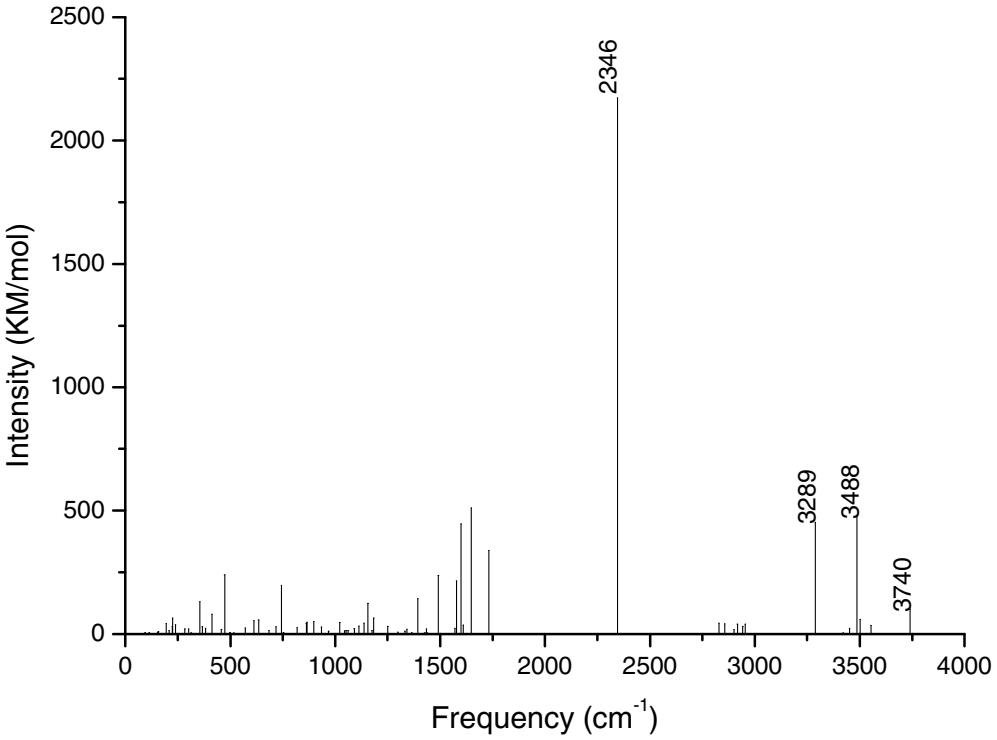
(C5-1)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