Supporting Information for

Kinetic Ion Thermometers for Electron Transfer Dissociation

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Complete references 18 and 19, Tables S1-S30, Figures S1-S7.

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Table S1. B3LYP/6-31+G(d,p) Optimized Structure of **1a**$^{2+}$ (**AALR_6-110)**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	7.749418	-1.025540	0.639247
2	1	0	8.164704	-1.959947	0.648990
3	1	0	8.410608	-0.373557	1.069116
4	1	0	7.543229	-0.730672	-0.363411
5	6	0	6.369839	-0.968671	1.270346
6	1	0	6.124033	-1.976624	1.615406
7	6	0	6.331734	0.028366	2.429135
8	1	0	7.020830	-0.270320	3.224591
9	1	0	5.330079	0.060826	2.864637
10	1	0	6.582804	1.039965	2.093590
11	6	0	5.462222	-0.589966	0.063219
12	8	0	6.020536	-0.369916	-1.023827
13	7	0	4.150100	-0.530172	0.273147

14	1	0	3.734260	-0.663141	1.194393
15	6	0	3.184408	-0.150187	-0.763164
16	1	0	3.587611	0.717157	-1.299153
17	6	0	2.925390	-1.293998	-1.761252
18	1	0	2.252174	-0.964157	-2.557960
19	1	0	2.474389	-2.156309	-1.262662
20	1	0	3.865561	-1.593374	-2.229328
21	6	0	1.909678	0.258775	0.002861
22	8	0	1.795920	0.026261	1.204695
23	7	0	0.927125	0.849651	-0.733776
24	1	0	1.144142	1.131137	-1.682070
25	6	0	-0.261510	1.441013	-0.110941
26	1	0	0.002664	1.710954	0.915525
27	6	0	-0.719738	2.694808	-0.887191
28	1	0	-0.928208	2.406168	-1.927990
29	1	0	-1.675058	3.011797	-0.455424
30	6	0	0.261267	3.887486	-0.869118
31	1	0	1.230600	3.551357	-1.268109
32	6	0	0.494931	4.432128	0.548544
33	1	0	0.941627	3.690834	1.220497
34	1	0	-0.447138	4.768705	0.997909
35	1	0	1.171178	5.291983	0.521408
36	6	0	-0.262109	4.992143	-1.801759
37	1	0	0.435430	5.834216	-1.837280
38	1	0	-1.227100	5.376991	-1.451280
39	1	0	-0.397479	4.627905	-2.826073
40	6	0	-1.429124	0.454149	0.042121
41	8	0	-2.395504	0.773546	0.760154
42	6	0	-1.388365	-3.091476	-0.358500
43	8	0	-0.228434	-3.124587	-0.715123
44	8	0	-2.068598	-4.144365	0.111126
45	1	0	-1.490036	-4.928178	0.102371
46	7	0	-1.364885	-0.706298	-0.634895
47	1	0	-0.485033	-0.933426	-1.087951
48	6	0	-2.265020	-1.836971	-0.424068
49	1	0	-2.750728	-1.718403	0.548861
50	6	0	-3.326160	-2.013706	-1.544259
51	1	0	-2.787640	-2.140029	-2.490687
52	1	0	-3.851851	-2.956174	-1.356234
53	6	0	-4.356565	-0.884507	-1.735058
54	1	0	-4.858907	-1.075426	-2.688991
55	1	0	-3.859563	0.086166	-1.851227
56	6	0	-5.468988	-0.769083	-0.680009
57	1	0	-6.283987	-0.162682	-1.094676
58	1	0	-5.868484	-1.766869	-0.452677
59	7	0	-4.974662	-0.134875	0.548272
60	1	0	-3.988915	0.176854	0.569584
61	6	0	-5.716133	0.219006	1.592584
62	7	0	-7.015488	-0.112101	1.675298
63	1	0	-7.594238	0.207216	2.437718
64	1	0	-7.461161	-0.666940	0.961408
65	7	0	-5.145242	0.925687	2.585158
66	1	0	-5.635731	1.134987	3.441005
67	1	0	-4.175127	1.203183	2.511876

Rotational constants (GHZ): 0.2054840 0.0671784 0.0579565

ZPVE = 1536.4992 kJ mol^{-1}

E[B3LYP/6-31+G(d,p)] = -1467.33295088 a.u.

E[B3LYP/6-311++G(2d,p)] = -1467.69131438 a.u.

E[MP2/6-311++G(2d,p)] = -1463.8663088 a.u.

Table S2. M06-2X/6-31+G(d,p) Optimized Structure of **1a**$^{2+}$ (**AALR_6-110)**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	7.417893	-1.372809	0.631961
2	1	0	7.751880	-2.296997	0.349065
3	1	0	8.091607	-0.973746	1.290732
4	1	0	7.336566	-0.755084	-0.224303
5	6	0	6.010365	-1.383197	1.172729
6	1	0	5.674934	-2.421837	1.224195
7	6	0	5.949814	-0.711637	2.539871
8	1	0	6.563097	-1.249782	3.266981
9	1	0	4.923357	-0.712818	2.911939
10	1	0	6.282883	0.328905	2.478478
11	6	0	5.216960	-0.616120	0.088397
12	8	0	5.852755	-0.109064	-0.838247
13	7	0	3.900584	-0.534220	0.237449
14	1	0	3.404261	-0.936584	1.029872
15	6	0	3.070663	0.214139	-0.700436
16	1	0	3.567576	1.170943	-0.901391
17	6	0	2.860099	-0.551608	-2.011449
18	1	0	2.278120	0.047924	-2.716875
19	1	0	2.327868	-1.487865	-1.823784
20	1	0	3.828548	-0.759003	-2.470767
21	6	0	1.745391	0.458743	0.023999
22	8	0	1.475537	-0.112244	1.070829
23	7	0	0.873426	1.301506	-0.588956
24	1	0	1.188345	1.854042	-1.376548
25	6	0	-0.352356	1.700110	0.088289
26	1	0	-0.126214	1.919172	1.137533
27	6	0	-0.976398	2.929128	-0.585901
28	1	0	-1.302390	2.658792	-1.600370
29	1	0	-1.878506	3.179212	-0.015302
30	6	0	-0.064920	4.164962	-0.646183
31	1	0	0.768147	3.963239	-1.337326
32	6	0	0.522037	4.512527	0.721865
33	1	0	1.198992	3.736381	1.095918
34	1	0	-0.275713	4.652900	1.460587
35	1	0	1.090476	5.444551	0.668144
36	6	0	-0.854436	5.342730	-1.220874
37	1	0	-0.210485	6.216310	-1.349370
38	1	0	-1.669040	5.624355	-0.544521
39	1	0	-1.290214	5.099292	-2.194740
40	6	0	-1.379619	0.574141	0.141108
41	8	0	-2.293569	0.629144	0.976038
42	6	0	-0.989646	-2.772257	-0.884417
43	8	0	0.151002	-2.596290	-1.241236
44	8	0	-1.527141	-3.963060	-0.632378
45	1	0	-0.867318	-4.656928	-0.797056
46	7	0	-1.274550	-0.400757	-0.774518
47	1	0	-0.431186	-0.416910	-1.340018
48	6	0	-2.009414	-1.650698	-0.711885
49	1	0	-2.449822	-1.748933	0.285905
50	6	0	-3.087259	-1.787044	-1.809159
51	1	0	-2.578959	-1.712547	-2.777592
52	1	0	-3.504834	-2.797708	-1.747091
53	6	0	-4.221877	-0.756238	-1.783392
54	1	0	-4.744517	-0.820059	-2.741734
55	1	0	-3.819105	0.263711	-1.724615
56	6	0	-5.272517	-0.949685	-0.687076

57	1	0	-6.164575	-0.361675	-0.935296
58	1	0	-5.558663	-2.008202	-0.626786
59	7	0	-4.737879	-0.505890	0.596453
60	1	0	-3.809303	-0.055775	0.615595
61	6	0	-5.378830	-0.519536	1.754100
62	7	0	-6.618680	-1.011443	1.854759
63	1	0	-7.105095	-1.039538	2.737969
64	1	0	-7.112285	-1.349309	1.043065
65	7	0	-4.751769	-0.042716	2.837652
66	1	0	-5.214454	0.034206	3.729803
67	1	0	-3.824163	0.353031	2.738533

Rotational constants (GHZ): 0.1967910 0.0733168 0.0627005

ZPVE = 1551.2482 kJ mol^{-1}

E[M06-2X/6-31+G(d,p)] = -1466.68365355 a.u.

E[M06-2X/6-311++G(2d,p)] = -1467.07329907 a.u.

Table S3. B3LYP/6-31+G(d,p) Optimized Structure of **$1b^{2+}$** (**AALR_6-61)**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-7.868025	-1.571951	-0.401882
2	1	0	-8.597983	-0.946891	-0.050353
3	1	0	-7.386076	-2.063483	0.410954
4	1	0	-8.303017	-2.260397	-1.020192
5	6	0	-6.712441	-0.825158	-1.043493
6	1	0	-6.589935	-1.218547	-2.056345
7	6	0	-6.972987	0.681118	-1.073304
8	1	0	-7.861960	0.912178	-1.667573
9	1	0	-6.130974	1.199900	-1.537982
10	1	0	-7.097696	1.085143	-0.063269
11	6	0	-5.501539	-1.257117	-0.164831
12	8	0	-5.733221	-2.002173	0.801814
13	7	0	-4.301092	-0.803604	-0.511523
14	1	0	-4.160358	-0.148389	-1.281275
15	6	0	-3.074286	-1.082402	0.241686
16	1	0	-3.297797	-0.976142	1.309262
17	6	0	-2.539503	-2.498760	-0.033822
18	1	0	-1.635537	-2.691152	0.551256
19	1	0	-2.299995	-2.622540	-1.093999
20	1	0	-3.288038	-3.240533	0.253366
21	6	0	-2.079862	0.015159	-0.197669
22	8	0	-2.328788	0.712846	-1.183035
23	7	0	-0.956357	0.136742	0.546973
24	1	0	-0.810992	-0.470224	1.343534
25	6	0	0.063547	1.148516	0.283782
26	1	0	-0.238401	1.648392	-0.638938
27	6	0	0.175537	2.176395	1.439152
28	1	0	0.398121	1.624347	2.361679
29	1	0	1.044955	2.818002	1.242625
30	6	0	-1.063757	3.070726	1.650929
31	1	0	-1.939111	2.415109	1.768554
32	6	0	-1.318856	4.010097	0.461497
33	1	0	-0.458933	4.669632	0.292207
34	1	0	-2.184651	4.649745	0.659550
35	1	0	-1.524418	3.468393	-0.467561
36	6	0	-0.899627	3.869035	2.954878
37	1	0	-1.781900	4.487709	3.145244
38	1	0	-0.033737	4.539446	2.899820

39	1	0	-0.760652	3.210399	3.819376
40	6	0	1.427353	0.477912	0.090874
41	8	0	1.778647	-0.471192	0.822118
42	6	0	4.282707	2.155543	-1.271336
43	8	0	3.647134	3.134815	-1.594484
44	8	0	5.614151	2.118697	-1.127764
45	1	0	5.980056	2.996986	-1.339599
46	7	0	2.211352	1.015058	-0.861295
47	1	0	1.875783	1.839777	-1.353020
48	6	0	3.648989	0.784602	-1.004667
49	1	0	4.040604	0.412836	-0.054299
50	6	0	4.013991	-0.181255	-2.163180
51	1	0	3.583952	0.230842	-3.083222
52	1	0	5.102020	-0.153332	-2.287719
53	6	0	3.553154	-1.643964	-2.033179
54	1	0	3.699834	-2.114595	-3.010848
55	1	0	2.475753	-1.700555	-1.835708
56	6	0	4.310025	-2.514524	-1.018142
57	1	0	4.103070	-3.570939	-1.231865
58	1	0	5.390296	-2.349690	-1.122835
59	7	0	3.898592	-2.206349	0.358272
60	1	0	3.071715	-1.600309	0.486685
61	6	0	4.476528	-2.665457	1.462514
62	7	0	4.027797	-2.241530	2.659593
63	1	0	4.346490	-2.655171	3.522513
64	1	0	3.262368	-1.582789	2.704761
65	7	0	5.505309	-3.527241	1.410847
66	1	0	5.827756	-3.907696	0.534684
67	1	0	5.999152	-3.810097	2.244313

Rotational constants (GHZ): 0.1937319 0.0638778 0.0559473

ZPVE = 1536.5493 kJ mol^{-1}

E[B3LYP/6-31+G(d,p)] = -1467.32969578 a.u.

E[B3LYP/6-311++G(2d,p)] = -1467.6883425 a.u.

E[MP2/6-311++G(2d,p)] = -1463.8616914 a.u.

Table S4. M06-2X/6-31+G(d,p) Optimized Structure of **$1b^{2+}$** (**AALR_6-61)**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-7.889395	-1.623405	-0.231930
2	1	0	-8.673392	-1.122967	0.194697
3	1	0	-7.369755	-2.184123	0.499348
4	1	0	-8.260651	-2.261912	-0.939163
5	6	0	-6.825648	-0.696299	-0.763254
6	1	0	-6.775714	-0.820154	-1.847666
7	6	0	-7.129406	0.748448	-0.382254
8	1	0	-8.070331	1.081770	-0.827353
9	1	0	-6.340304	1.405718	-0.753117
10	1	0	-7.177806	0.862383	0.705064
11	6	0	-5.535327	-1.228816	-0.096278
12	8	0	-5.650402	-2.110804	0.758178
13	7	0	-4.389448	-0.678917	-0.474919
14	1	0	-4.332948	0.068420	-1.165654
15	6	0	-3.110812	-1.051316	0.121252
16	1	0	-3.230857	-1.062450	1.211029
17	6	0	-2.638535	-2.424276	-0.366826
18	1	0	-1.695359	-2.700472	0.111228
19	1	0	-2.491312	-2.410711	-1.449991

20	1	0	-3.382800	-3.180855	-0.110591
21	6	0	-2.136536	0.061921	-0.287344
22	8	0	-2.458173	0.883455	-1.137676
23	7	0	-0.932579	0.048678	0.320539
24	1	0	-0.707941	-0.649032	1.019383
25	6	0	0.082769	1.045878	0.031564
26	1	0	-0.153258	1.469470	-0.949827
27	6	0	0.127685	2.162974	1.096162
28	1	0	0.291379	1.687525	2.072610
29	1	0	0.999867	2.802548	0.898778
30	6	0	-1.127083	3.044164	1.141401
31	1	0	-2.004074	2.390009	1.254588
32	6	0	-1.288391	3.863806	-0.139919
33	1	0	-0.405403	4.492764	-0.305789
34	1	0	-2.152233	4.529658	-0.059756
35	1	0	-1.446297	3.233994	-1.020062
36	6	0	-1.053720	3.960433	2.364989
37	1	0	-1.945575	4.589023	2.432191
38	1	0	-0.185204	4.625293	2.297361
39	1	0	-0.971283	3.389119	3.294808
40	6	0	1.443853	0.367970	-0.002000
41	8	0	1.678584	-0.622396	0.711698
42	6	0	4.451169	2.096601	-0.628316
43	8	0	3.865870	3.125521	-0.851038
44	8	0	5.744137	2.002047	-0.322752
45	1	0	6.138111	2.891091	-0.322074
46	7	0	2.358866	0.948864	-0.790959
47	1	0	2.100718	1.816974	-1.254454
48	6	0	3.793108	0.720028	-0.703445
49	1	0	4.006590	0.192917	0.231329
50	6	0	4.361731	-0.040852	-1.919782
51	1	0	4.113852	0.543382	-2.813372
52	1	0	5.453945	-0.040175	-1.836018
53	6	0	3.858268	-1.473428	-2.121934
54	1	0	4.141520	-1.788765	-3.130042
55	1	0	2.760855	-1.506824	-2.092612
56	6	0	4.426757	-2.508789	-1.149197
57	1	0	4.237186	-3.519528	-1.527452
58	1	0	5.510611	-2.370673	-1.052187
59	7	0	3.803580	-2.346609	0.163815
60	1	0	2.919632	-1.828124	0.212040
61	6	0	4.327807	-2.674546	1.333818
62	7	0	3.738716	-2.220151	2.449213
63	1	0	3.960999	-2.602090	3.355679
64	1	0	2.938271	-1.603853	2.365002
65	7	0	5.437177	-3.416769	1.415434
66	1	0	5.805518	-3.892356	0.605803
67	1	0	5.898747	-3.574818	2.298796

Rotational constants (GHZ): 0.2143466 0.0640755 0.0550157

ZPVE = 1552.125 kJ mol^{-1}

E[M06-2X/6-31+G(d,p)] = -1466.67887809 a.u.

E[M06-2X/6-311++G(2d,p)] = -1467.06862105 a.u.

Table S5. B3LYP/6-31+G(d,p) Optimized Structure of **1c^{2+}** (**AALR_4-837)**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-3.759140	-3.006189	0.691840
2	1	0	-4.301008	-3.872959	0.740530
3	1	0	-3.706442	-2.585420	1.627965
4	1	0	-2.761195	-3.239419	0.436568
5	6	0	-4.396352	-2.016939	-0.253713
6	1	0	-4.182478	-2.376914	-1.264404
7	6	0	-5.905894	-1.942395	-0.001873
8	1	0	-6.377244	-2.917553	-0.158607
9	1	0	-6.371461	-1.243390	-0.700488
10	1	0	-6.126245	-1.597975	1.013538
11	6	0	-3.666444	-0.677694	-0.010753
12	8	0	-2.927479	-0.550997	0.972265
13	7	0	-3.902900	0.299680	-0.905454
14	1	0	-4.421627	0.080099	-1.745609
15	6	0	-3.258526	1.624035	-0.839258
16	1	0	-3.540300	2.123766	-1.772426
17	6	0	-3.766982	2.465246	0.336911
18	1	0	-4.856111	2.537706	0.287512
19	1	0	-3.381853	3.488060	0.274956
20	1	0	-3.498091	2.028361	1.301373
21	6	0	-1.729070	1.431743	-0.963006
22	8	0	-1.274991	0.669633	-1.829449
23	7	0	-0.917727	2.109746	-0.123669
24	1	0	-1.320902	2.745120	0.551941
25	6	0	0.541577	2.108531	-0.282363
26	1	0	0.787236	2.467288	-1.286906
27	6	0	1.209724	3.014274	0.774116
28	1	0	0.968583	2.630425	1.775102
29	1	0	2.292769	2.906142	0.646646
30	6	0	0.850366	4.516234	0.695999
31	1	0	-0.236124	4.630509	0.838969
32	6	0	1.218634	5.141791	-0.657733
33	1	0	0.985768	6.210543	-0.659454
34	1	0	0.674650	4.693923	-1.496806
35	1	0	2.291999	5.039119	-0.857205
36	6	0	1.537659	5.259385	1.853512
37	1	0	1.261257	6.317584	1.852129
38	1	0	2.628656	5.202203	1.761890
39	1	0	1.258194	4.842512	2.827177
40	6	0	1.134425	0.695605	-0.241218
41	8	0	2.211992	0.471976	-0.813109
42	6	0	-0.559531	-2.384166	-0.151425
43	8	0	-1.038729	-3.338022	0.449026
44	8	0	-1.190074	-1.915184	-1.221112
45	1	0	-0.942497	-1.001200	-1.521979
46	7	0	0.463621	-0.264294	0.443193
47	1	0	-0.403218	-0.000301	0.901742
48	6	0	0.746738	-1.695455	0.290717
49	1	0	1.435933	-1.783084	-0.556292
50	6	0	1.342533	-2.357781	1.545179
51	1	0	0.623572	-2.243759	2.363415
52	1	0	1.410510	-3.434514	1.357015
53	6	0	2.706556	-1.823382	2.024943
54	1	0	2.862873	-2.216804	3.034296
55	1	0	2.684065	-0.732158	2.134425
56	6	0	3.949909	-2.230313	1.215725

57	1	0	4.838246	-2.048377	1.833144
58	1	0	3.908619	-3.303717	0.986740
59	7	0	4.067122	-1.459147	-0.029961
60	1	0	3.349069	-0.752214	-0.238152
61	6	0	5.101990	-1.488655	-0.867892
62	7	0	5.117213	-0.640282	-1.910512
63	1	0	4.365370	0.025451	-2.033580
64	1	0	5.851922	-0.657075	-2.601521
65	7	0	6.118647	-2.347193	-0.692808
66	1	0	6.126687	-3.004051	0.071963
67	1	0	6.923347	-2.343796	-1.302175

Rotational constants (GHZ): 0.1706678 0.1090275 0.0755758

ZPVE = 1541.192 kJ mol^{-1}

E[B3LYP/6-31+G(d,p)] = -1467.3304708 a.u.

E[B3LYP/6-311++G(2d,p)] = -1467.68744475 a.u.

E[MP2/6-311++G(2d,p)] = -1463.873803 a.u.

Table S6. M06-2X/6-31+G(d,p) Optimized Structure of **$1c^{2+}$** (**AALR_4-837)**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-3.559433	-3.060570	0.727852
2	1	0	-4.100405	-3.926116	0.798562
3	1	0	-3.500878	-2.622976	1.655572
4	1	0	-2.561071	-3.298139	0.468069
5	6	0	-4.197047	-2.104285	-0.231602
6	1	0	-3.975328	-2.473985	-1.237655
7	6	0	-5.700889	-2.033014	0.022779
8	1	0	-6.164090	-3.014915	-0.104365
9	1	0	-6.176983	-1.356646	-0.689327
10	1	0	-5.912387	-1.663143	1.030599
11	6	0	-3.493668	-0.755951	-0.020627
12	8	0	-2.676509	-0.613831	0.890322
13	7	0	-3.849373	0.223920	-0.862418
14	1	0	-4.433137	0.009087	-1.659559
15	6	0	-3.258441	1.560447	-0.778943
16	1	0	-3.587648	2.089193	-1.679598
17	6	0	-3.734265	2.322296	0.455751
18	1	0	-4.825347	2.351863	0.464018
19	1	0	-3.390732	3.360559	0.426989
20	1	0	-3.393849	1.844108	1.377502
21	6	0	-1.738275	1.414878	-0.945842
22	8	0	-1.280593	0.664610	-1.809534
23	7	0	-0.933346	2.125380	-0.133996
24	1	0	-1.328207	2.753432	0.553210
25	6	0	0.508251	2.136462	-0.342375
26	1	0	0.725074	2.504960	-1.351411
27	6	0	1.202984	3.018391	0.703753
28	1	0	1.070471	2.570842	1.698846
29	1	0	2.275834	2.993120	0.478129
30	6	0	0.735000	4.482876	0.723761
31	1	0	-0.307622	4.523279	1.077172
32	6	0	0.799340	5.123218	-0.662852
33	1	0	0.556507	6.187043	-0.603270
34	1	0	0.097412	4.668839	-1.370507
35	1	0	1.809149	5.036880	-1.080908
36	6	0	1.582528	5.262991	1.731004
37	1	0	1.229483	6.293283	1.817894

38	1	0	2.628690	5.294237	1.407487
39	1	0	1.546693	4.809168	2.726147
40	6	0	1.100886	0.733957	-0.315523
41	8	0	2.166429	0.516515	-0.900063
42	6	0	-0.480596	-2.377764	-0.144292
43	8	0	-0.895804	-3.351984	0.458624
44	8	0	-1.144324	-1.938513	-1.197919
45	1	0	-0.911632	-1.029313	-1.507164
46	7	0	0.452122	-0.217664	0.392129
47	1	0	-0.425323	0.032236	0.843670
48	6	0	0.786423	-1.632196	0.289306
49	1	0	1.498740	-1.729012	-0.539118
50	6	0	1.353748	-2.228790	1.581221
51	1	0	0.593263	-2.113946	2.361146
52	1	0	1.474398	-3.307139	1.434046
53	6	0	2.666724	-1.614121	2.082131
54	1	0	2.804856	-1.933470	3.118614
55	1	0	2.598278	-0.518335	2.112133
56	6	0	3.933760	-2.020226	1.324645
57	1	0	4.810933	-1.752986	1.926208
58	1	0	3.940033	-3.106019	1.162478
59	7	0	3.995968	-1.331670	0.037414
60	1	0	3.305934	-0.598900	-0.162619
61	6	0	4.937452	-1.485277	-0.884303
62	7	0	4.846480	-0.777659	-2.016849
63	1	0	4.077402	-0.129707	-2.140124
64	1	0	5.578257	-0.787886	-2.710651
65	7	0	5.945768	-2.343240	-0.703509
66	1	0	6.061166	-2.837618	0.167899
67	1	0	6.647670	-2.489084	-1.413851

Rotational constants (GHZ): 0.1722502 0.1154109 0.0790770

ZPVE = 1556.4556 kJ mol^{-1}

E[M06-2X/6-31+G(d,p)] = -1466.69525193 a.u.

E[M06-2X/6-311++G(2d,p)] = -1467.08309461 a.u.

Table S7. B3LYP/6-31+G(d,p) Optimized Structure of **$1d^{2+}$** (**AALR_7-833)**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-3.656761	-2.788070	1.089531
2	1	0	-2.665286	-3.035139	0.821890
3	1	0	-4.166808	-3.649900	1.300710
4	1	0	-3.571977	-2.227327	1.946187
5	6	0	-4.373982	-1.975603	0.038656
6	1	0	-4.217877	-2.496542	-0.910763
7	6	0	-5.865478	-1.878273	0.375968
8	1	0	-6.323528	-2.871398	0.414625
9	1	0	-6.391641	-1.310782	-0.395021
10	1	0	-6.026920	-1.372676	1.333338
11	6	0	-3.661331	-0.605687	0.007185
12	8	0	-2.861399	-0.309275	0.902499
13	7	0	-3.980226	0.206744	-1.016629
14	1	0	-4.552458	-0.153679	-1.768824
15	6	0	-3.366199	1.532890	-1.213239
16	1	0	-3.702513	1.857642	-2.203832
17	6	0	-3.839989	2.556988	-0.175826
18	1	0	-3.520124	2.295691	0.835637
19	1	0	-4.931439	2.606987	-0.186091
20	1	0	-3.478070	3.558484	-0.429173

21	6	0	-1.840356	1.346216	-1.376324
22	8	0	-1.408136	0.451810	-2.118820
23	7	0	-1.007100	2.174360	-0.711355
24	1	0	-1.387826	2.903387	-0.124042
25	6	0	0.439725	2.165105	-0.965773
26	1	0	0.580693	2.245669	-2.049648
27	6	0	1.171042	3.361294	-0.312870
28	1	0	2.149577	3.407058	-0.801030
29	1	0	0.642163	4.274512	-0.617228
30	6	0	1.390153	3.366384	1.216459
31	1	0	1.902408	2.430798	1.488551
32	6	0	0.094170	3.453039	2.041652
33	1	0	-0.490235	4.341377	1.767705
34	1	0	0.325011	3.543383	3.107305
35	1	0	-0.543669	2.568460	1.932378
36	6	0	2.329050	4.529949	1.579589
37	1	0	2.545266	4.536380	2.652068
38	1	0	1.874262	5.495376	1.328682
39	1	0	3.282246	4.461612	1.045150
40	6	0	1.096269	0.818301	-0.633827
41	8	0	2.185446	0.536023	-1.156586
42	6	0	-0.509252	-2.247991	0.020741
43	8	0	-0.942525	-3.100138	0.786594
44	8	0	-1.176321	-1.988588	-1.096379
45	1	0	-0.975473	-1.127664	-1.549718
46	7	0	0.453693	-0.028270	0.207047
47	1	0	-0.420716	0.284794	0.617963
48	6	0	0.781115	-1.454721	0.308872
49	1	0	1.464028	-1.673748	-0.519574
50	6	0	1.409104	-1.865501	1.652704
51	1	0	0.694109	-1.627322	2.447315
52	1	0	1.507149	-2.956217	1.657884
53	6	0	2.760351	-1.217506	2.012325
54	1	0	2.934618	-1.417716	3.074232
55	1	0	2.706721	-0.125520	1.923093
56	6	0	4.008790	-1.730368	1.274877
57	1	0	4.896468	-1.418572	1.839274
58	1	0	3.994813	-2.828116	1.240967
59	7	0	4.094228	-1.191441	-0.089529
60	1	0	3.362253	-0.539819	-0.403885
61	6	0	5.113885	-1.362181	-0.929202
62	7	0	6.149606	-2.156750	-0.617235
63	1	0	6.188416	-2.649254	0.261549
64	1	0	6.936666	-2.267567	-1.239486
65	7	0	5.093010	-0.728257	-2.114429
66	1	0	5.828109	-0.845056	-2.795249
67	1	0	4.327505	-0.108479	-2.345023

Rotational constants (GHZ): 0.1998731 0.1041411 0.0819942

ZPVE = 1541.3443 kJ mol^{-1}

E[B3LYP/6-31+G(d,p)] = -1467.32683186 a.u.

E[B3LYP/6-311++G(2d,p)] = -1467.68361678 a.u.

E[MP2/6-311++G(2d,p)] = -1463.8727867 a.u.

Table S8. M06-2X/6-31+G(d,p) Optimized Structure of **1d^{2+}** (**AALR_7-833)**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-3.519073	-2.770933	1.114804
2	1	0	-2.527369	-3.034853	0.855282
3	1	0	-4.040673	-3.622185	1.339045
4	1	0	-3.434225	-2.196555	1.962144
5	6	0	-4.210391	-1.983980	0.044972
6	1	0	-4.024919	-2.508322	-0.897938
7	6	0	-5.702827	-1.885574	0.351112
8	1	0	-6.154286	-2.879607	0.406700
9	1	0	-6.221283	-1.340490	-0.439477
10	1	0	-5.877178	-1.358754	1.294073
11	6	0	-3.516640	-0.615005	0.003237
12	8	0	-2.649290	-0.328627	0.830869
13	7	0	-3.935590	0.218822	-0.958222
14	1	0	-4.561788	-0.122843	-1.674807
15	6	0	-3.351601	1.549541	-1.131830
16	1	0	-3.744100	1.925987	-2.082099
17	6	0	-3.750021	2.503178	-0.007250
18	1	0	-3.327790	2.190621	0.951404
19	1	0	-4.837571	2.521719	0.083639
20	1	0	-3.434512	3.525133	-0.236127
21	6	0	-1.843973	1.375506	-1.367663
22	8	0	-1.429443	0.479855	-2.106262
23	7	0	-1.003655	2.224524	-0.751371
24	1	0	-1.363282	2.953401	-0.150352
25	6	0	0.425158	2.193420	-1.038849
26	1	0	0.556804	2.291820	-2.122648
27	6	0	1.182972	3.335374	-0.342434
28	1	0	2.156986	3.403815	-0.836691
29	1	0	0.657769	4.273150	-0.569322
30	6	0	1.407293	3.214486	1.172145
31	1	0	1.964361	2.283213	1.358182
32	6	0	0.112306	3.167369	1.991712
33	1	0	-0.518572	4.038948	1.769788
34	1	0	0.337540	3.204861	3.060840
35	1	0	-0.474649	2.257714	1.820584
36	6	0	2.278313	4.384327	1.637198
37	1	0	2.508608	4.300343	2.702334
38	1	0	1.758508	5.336443	1.483520
39	1	0	3.222750	4.425404	1.087341
40	6	0	1.057588	0.842656	-0.718805
41	8	0	2.137339	0.551772	-1.243377
42	6	0	-0.486896	-2.215657	0.020146
43	8	0	-0.863446	-3.082442	0.789832
44	8	0	-1.190521	-1.970813	-1.069482
45	1	0	-0.997066	-1.118652	-1.532037
46	7	0	0.418656	0.016953	0.136974
47	1	0	-0.464255	0.325961	0.538406
48	6	0	0.775470	-1.388327	0.287037
49	1	0	1.477578	-1.625302	-0.522254
50	6	0	1.367547	-1.733776	1.657820
51	1	0	0.615875	-1.481871	2.414076
52	1	0	1.495446	-2.819940	1.709349
53	6	0	2.680772	-1.031016	2.021280
54	1	0	2.831650	-1.154064	3.097141
55	1	0	2.602987	0.050962	1.850368
56	6	0	3.942459	-1.562301	1.335943
57	1	0	4.824766	-1.192465	1.872627

58	1	0	3.950143	-2.659722	1.368488
59	7	0	3.990365	-1.109074	-0.051971
60	1	0	3.286559	-0.432049	-0.370152
61	6	0	4.944885	-1.387980	-0.929575
62	7	0	5.967762	-2.184889	-0.606775
63	1	0	6.073656	-2.547194	0.328423
64	1	0	6.685115	-2.419446	-1.276783
65	7	0	4.855264	-0.869497	-2.160425
66	1	0	5.586245	-0.991733	-2.844297
67	1	0	4.082483	-0.256206	-2.389668

Rotational constants (GHZ): 0.2065446 0.1095238 0.0865761

ZPVE = 1555.6688 kJ mol^{-1}

E[M06-2X/6-31+G(d,p)] = -1466.69439126 a.u.

E[M06-2X/6-311++G(2d,p)] = -1467.08206881 a.u.

Table S9. B3LYP/6-31+G(d,p) Optimized Structure of **2a**$^{2+}$ (**AAALR_5-171)**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.959248	0.655283	-2.777917
2	1	0	3.046401	1.002611	-3.735766
3	1	0	3.576401	1.197010	-2.162993
4	1	0	1.960974	0.808916	-2.422940
5	6	0	3.342068	-0.797614	-2.682532
6	6	0	4.727554	-1.038319	-3.290091
7	6	0	3.277624	-1.120814	-1.176481
8	8	0	3.349940	-0.193397	-0.361032
9	7	0	3.158229	-2.415396	-0.838128
10	1	0	3.003317	-3.100691	-1.565352
11	6	0	3.021547	-2.864777	0.561690
12	6	0	4.334757	-2.744283	1.341403
13	6	0	1.767623	-2.178938	1.159528
14	8	0	0.679023	-2.283586	0.591201
15	7	0	1.914021	-1.462478	2.301658
16	1	0	2.821328	-1.386587	2.740334
17	6	0	0.765207	-0.833938	2.947863
18	6	0	1.182746	-0.189684	4.276702
19	6	0	0.067129	0.188438	2.036262
20	8	0	-1.158107	0.384458	2.162251
21	7	0	0.813145	0.874407	1.151939
22	1	0	1.775358	0.588876	0.989195
23	6	0	0.225839	1.864735	0.244127
24	6	0	1.230300	2.976372	-0.097236
25	6	0	1.600861	3.904462	1.080917
26	6	0	-0.304465	1.159768	-1.022850
27	8	0	0.435296	0.815220	-1.970913
28	6	0	-3.758283	0.973582	-2.146600
29	8	0	-4.247349	1.437247	-1.135841
30	8	0	-4.399531	0.844264	-3.312685
31	1	0	-5.300778	1.205316	-3.227514
32	7	0	-1.625049	0.928756	-1.050995
33	1	0	-2.209088	1.286053	-0.300992
34	6	0	-2.335076	0.428262	-2.227263
35	6	0	-2.317311	-1.115744	-2.420880
36	6	0	-3.293938	-1.997971	-1.613078
37	6	0	-2.900132	-2.386733	-0.176298
38	7	0	-3.039181	-1.332805	0.835994

39	1	0	-2.200549	-0.829793	1.123886
40	6	0	-4.120009	-1.076065	1.575284
41	7	0	-4.009255	-0.234245	2.614602
42	1	0	-3.100882	0.165026	2.831499
43	1	0	-4.825498	0.144231	3.070926
44	7	0	-5.304699	-1.652841	1.313473
45	1	0	-6.085483	-1.549183	1.944316
46	1	0	-5.442837	-2.232011	0.501081
47	6	0	2.771475	4.812982	0.672339
48	6	0	0.406173	4.743074	1.563444
49	1	0	2.573473	-1.354281	-3.227047
50	1	0	5.498722	-0.473653	-2.756673
51	1	0	4.745904	-0.756473	-4.347367
52	1	0	4.985379	-2.098460	-3.229925
53	1	0	2.746414	-3.921775	0.496844
54	1	0	4.675766	-1.708555	1.416187
55	1	0	5.114808	-3.319973	0.836954
56	1	0	4.224703	-3.167263	2.344854
57	1	0	0.006097	-1.599774	3.136214
58	1	0	1.951439	0.575682	4.128501
59	1	0	1.568715	-0.951991	4.959610
60	1	0	0.319071	0.280394	4.751695
61	1	0	-0.628496	2.294423	0.770346
62	1	0	2.143073	2.512875	-0.492227
63	1	0	0.806902	3.581635	-0.909321
64	1	0	1.939452	3.275578	1.916541
65	1	0	-1.852758	0.859557	-3.110107
66	1	0	-2.538749	-1.278012	-3.480310
67	1	0	-1.286738	-1.450755	-2.262371
68	1	0	-3.376556	-2.944382	-2.160663
69	1	0	-4.302618	-1.565247	-1.628449
70	1	0	-3.491445	-3.252604	0.142782
71	1	0	-1.852694	-2.699725	-0.142938
72	1	0	2.492272	5.463855	-0.165077
73	1	0	3.071559	5.458311	1.502959
74	1	0	3.650523	4.231034	0.371843
75	1	0	0.023320	5.380766	0.757363
76	1	0	-0.423286	4.130108	1.933495
77	1	0	0.707567	5.399755	2.384879

Rotational constants (GHZ): 0.1297541 0.0833021 0.0818962

ZPVE = 1763.0822 kJ mol^{-1}

E[B3LYP/6-31+G(d,p)] = -1714.69044585 a.u.

E[B3LYP/6-311++G(2d,p)] = -1715.10767486 a.u.

E[MP2/6-311++G(2d,p)] = -1710.6695901 a.u.

Table S10. M06-2X/6-31+G(d,p) Optimized Structure of **2a^{2+}** (**AAALR_5-171)**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	3.048422	-0.986037	-2.555575
2	1	0	3.246490	-1.140930	-3.546004
3	1	0	3.789352	-0.407323	-2.147104
4	1	0	2.104279	-0.470649	-2.422945
5	6	0	2.956556	-2.272539	-1.805152
6	6	0	4.230811	-3.097454	-1.963944
7	6	0	2.716075	-1.862431	-0.348560
8	8	0	2.992530	-0.719344	0.014051
9	7	0	2.243960	-2.809312	0.473915

10	1	0	1.967920	-3.706757	0.100072
11	6	0	2.028177	-2.543225	1.898274
12	6	0	3.345710	-2.430219	2.660816
13	6	0	1.062350	-1.350838	2.017662
14	8	0	-0.005498	-1.354219	1.405388
15	7	0	1.421349	-0.318316	2.806351
16	1	0	2.315060	-0.316251	3.279075
17	6	0	0.523095	0.814997	2.974815
18	6	0	1.188195	1.912078	3.802316
19	6	0	0.083976	1.354827	1.614325
20	8	0	-1.072940	1.763039	1.448113
21	7	0	1.003740	1.395657	0.640836
22	1	0	1.879524	0.892404	0.763207
23	6	0	0.639113	1.797343	-0.710814
24	6	0	1.850684	2.339990	-1.460990
25	6	0	2.502435	3.560514	-0.793460
26	6	0	-0.012370	0.603787	-1.422552
27	8	0	0.638852	-0.229576	-2.085776
28	6	0	-3.498828	0.023217	-2.210887
29	8	0	-3.978037	0.900997	-1.531799
30	8	0	-4.150077	-0.636600	-3.164198
31	1	0	-5.047699	-0.275303	-3.257878
32	7	0	-1.334056	0.488320	-1.296040
33	1	0	-1.851248	1.186142	-0.766989
34	6	0	-2.085544	-0.504561	-2.047835
35	6	0	-2.081083	-1.939753	-1.454158
36	6	0	-3.223164	-2.338523	-0.504804
37	6	0	-3.041388	-1.942882	0.960594
38	7	0	-2.985825	-0.502579	1.196744
39	1	0	-2.068494	-0.079565	1.317760
40	6	0	-4.048497	0.289684	1.329629
41	7	0	-3.886087	1.572711	1.653371
42	1	0	-2.946657	1.939747	1.775168
43	1	0	-4.656298	2.220047	1.588083
44	7	0	-5.284241	-0.199919	1.175089
45	1	0	-6.093555	0.383302	1.323231
46	1	0	-5.444174	-1.147224	0.874109
47	6	0	3.655715	4.057162	-1.667157
48	6	0	1.493821	4.680656	-0.533224
49	1	0	2.082067	-2.799815	-2.199162
50	1	0	5.094017	-2.561457	-1.557972
51	1	0	4.416480	-3.329206	-3.015841
52	1	0	4.138833	-4.045066	-1.429252
53	1	0	1.461614	-3.398108	2.280264
54	1	0	3.948057	-1.592869	2.298550
55	1	0	3.921424	-3.347954	2.526673
56	1	0	3.164665	-2.319458	3.733661
57	1	0	-0.397880	0.476901	3.462872
58	1	0	2.103193	2.267195	3.318414
59	1	0	1.430362	1.540723	4.801165
60	1	0	0.505757	2.757031	3.911864
61	1	0	-0.116483	2.581345	-0.615032
62	1	0	2.599628	1.542523	-1.552439
63	1	0	1.533115	2.606850	-2.477671
64	1	0	2.918194	3.239751	0.171795
65	1	0	-1.631801	-0.563730	-3.042032
66	1	0	-2.114479	-2.619200	-2.310106
67	1	0	-1.112226	-2.080475	-0.959897
68	1	0	-3.299971	-3.431009	-0.520895
69	1	0	-4.183592	-1.976562	-0.894968
70	1	0	-3.836154	-2.375608	1.579186
71	1	0	-2.096154	-2.340060	1.333065
72	1	0	3.283281	4.418478	-2.632263

73	1	0	4.181249	4.884171	-1.183682
74	1	0	4.387942	3.265489	-1.859347
75	1	0	0.970844	4.956628	-1.456985
76	1	0	0.745183	4.402517	0.216642
77	1	0	2.003826	5.574299	-0.164811

Rotational constants (GHZ): 0.1381348 0.0930950 0.0888645

ZPVE = 1780.6943 kJ mol^{-1}

E[M06-2X/6-31+G(d,p)] = -1713.95771251 a.u.

E[M06-2X/6-311++G(2d,p)] = -1714.41021945 a.u.

Table S11. B3LYP/6-31+G(d,p) Optimized Structure of **2b**$^{2+}$ (**AAALR_6-844)**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.592933	1.599602	-2.513229
2	1	0	3.292482	1.854118	-1.807071
3	1	0	1.634809	1.626651	-2.029150
4	1	0	2.620557	2.278623	-3.277354
5	6	0	2.888595	0.207128	-3.000206
6	6	0	4.197521	0.170138	-3.795502
7	6	0	2.939168	-0.649689	-1.719877
8	8	0	3.197342	-0.103951	-0.641028
9	7	0	2.704261	-1.966335	-1.863596
10	1	0	2.423656	-2.318350	-2.769093
11	6	0	2.689866	-2.913699	-0.730593
12	6	0	4.088144	-3.157509	-0.154181
13	6	0	1.584085	-2.468077	0.257378
14	8	0	0.404646	-2.434734	-0.117678
15	7	0	1.949422	-2.115088	1.507093
16	1	0	2.926833	-2.127630	1.765619
17	6	0	0.963323	-1.687694	2.497224
18	6	0	1.641447	-1.432878	3.849883
19	6	0	0.166533	-0.451973	2.035914
20	8	0	-1.034328	-0.350330	2.331540
21	7	0	0.835515	0.516222	1.373489
22	1	0	1.774097	0.325953	1.034404
23	6	0	0.192525	1.766620	0.959237
24	6	0	1.191905	2.935132	0.940841
25	6	0	1.727952	3.368292	2.323684
26	6	0	-0.481279	1.577830	-0.414939
27	8	0	0.172811	1.441455	-1.475522
28	6	0	-3.763986	2.527015	-1.420382
29	8	0	-4.067617	3.029333	-0.360545
30	8	0	-4.338738	2.805963	-2.597674
31	1	0	-5.041503	3.467495	-2.460315
32	7	0	-1.817551	1.549405	-0.396617
33	1	0	-2.290393	1.724116	0.484681
34	6	0	-2.695726	1.438867	-1.558980
35	6	0	-3.381323	0.050059	-1.610150
36	6	0	-2.431325	-1.101911	-1.986749
37	6	0	-2.862532	-2.455954	-1.397803
38	7	0	-2.566871	-2.505113	0.041812
39	1	0	-1.588179	-2.346691	0.284099
40	6	0	-3.423959	-2.693624	1.049034
41	7	0	-3.064320	-2.335159	2.287980
42	1	0	-2.311412	-1.649735	2.432908
43	1	0	-3.602716	-2.640463	3.085607
44	7	0	-4.642389	-3.226808	0.833209

45	1	0	-5.340063	-3.226931	1.562955
46	1	0	-4.826942	-3.799768	0.023770
47	6	0	2.855479	4.396211	2.135825
48	6	0	0.621987	3.932378	3.229783
49	1	0	2.040854	-0.085636	-3.626749
50	1	0	5.047231	0.473481	-3.176004
51	1	0	4.141472	0.825501	-4.670088
52	1	0	4.389590	-0.842710	-4.158119
53	1	0	2.312311	-3.851389	-1.147960
54	1	0	4.540577	-2.242881	0.237854
55	1	0	4.743925	-3.544544	-0.938079
56	1	0	4.048460	-3.912896	0.636504
57	1	0	0.218653	-2.481552	2.609890
58	1	0	2.407075	-0.653926	3.775269
59	1	0	2.105596	-2.352185	4.218749
60	1	0	0.900014	-1.111868	4.584833
61	1	0	-0.589606	1.964634	1.694515
62	1	0	2.037638	2.662839	0.295360
63	1	0	0.699712	3.793686	0.465330
64	1	0	2.157863	2.483880	2.815367
65	1	0	-2.103720	1.612874	-2.460020
66	1	0	-3.825762	-0.125429	-0.622568
67	1	0	-4.209153	0.096862	-2.325158
68	1	0	-1.410552	-0.896001	-1.647386
69	1	0	-2.383479	-1.200427	-3.077123
70	1	0	-3.932440	-2.614907	-1.553200
71	1	0	-2.328087	-3.273843	-1.890375
72	1	0	2.485489	5.301311	1.639306
73	1	0	3.271036	4.698345	3.101457
74	1	0	3.677902	3.991438	1.534451
75	1	0	0.147155	4.808550	2.771927
76	1	0	-0.161783	3.199926	3.451446
77	1	0	1.040498	4.250551	4.189138

Rotational constants (GHZ): 0.1140548 0.0923956 0.0816214

ZPVE = 1763.5978 kJ mol^{-1}

E[B3LYP/6-31+G(d,p)] = -1714.69229479 a.u.

E[B3LYP/6-311++G(2d,p)] = -1715.10961569 a.u.

E[MP2/6-311++G(2d,p)] = -1710.6704502 a.u.

Table S12. M06-2X/6-31+G(d,p) Optimized Structure of **$2b^{2+}$** (**AAALR_6-844)**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.631871	1.662552	-2.401479
2	1	0	3.386594	1.825409	-1.727733
3	1	0	1.682669	1.726863	-1.866573
4	1	0	2.677456	2.373276	-3.134447
5	6	0	2.762957	0.288492	-2.966299
6	6	0	4.047698	0.145215	-3.778125
7	6	0	2.738911	-0.642811	-1.750351
8	8	0	2.943809	-0.181532	-0.627868
9	7	0	2.520795	-1.943640	-1.989694
10	1	0	2.272848	-2.247191	-2.921152
11	6	0	2.461585	-2.915364	-0.894811
12	6	0	3.834688	-3.171145	-0.280270
13	6	0	1.353531	-2.458473	0.070225
14	8	0	0.226281	-2.209658	-0.357009
15	7	0	1.652128	-2.336291	1.378184

16	1	0	2.587725	-2.519992	1.715018
17	6	0	0.624715	-1.913206	2.315626
18	6	0	1.197566	-1.808277	3.727561
19	6	0	0.014470	-0.571372	1.902037
20	8	0	-1.178917	-0.333826	2.122570
21	7	0	0.846160	0.338982	1.373586
22	1	0	1.763937	0.051398	1.044714
23	6	0	0.390609	1.680216	1.042045
24	6	0	1.559481	2.662824	1.039345
25	6	0	2.344517	2.708236	2.359729
26	6	0	-0.336798	1.645962	-0.305460
27	8	0	0.269867	1.566130	-1.396285
28	6	0	-3.624584	2.750178	-1.096541
29	8	0	-3.885968	3.128010	0.017430
30	8	0	-4.258873	3.125976	-2.204548
31	1	0	-4.964343	3.753778	-1.972906
32	7	0	-1.662616	1.678750	-0.242434
33	1	0	-2.106007	1.750700	0.669585
34	6	0	-2.552966	1.707938	-1.390741
35	6	0	-3.233009	0.342363	-1.593821
36	6	0	-2.246655	-0.767368	-1.966893
37	6	0	-2.721014	-2.140159	-1.485971
38	7	0	-2.652427	-2.192143	-0.024565
39	1	0	-1.736634	-1.964058	0.359538
40	6	0	-3.658678	-2.332548	0.832064
41	7	0	-3.480569	-1.987425	2.108148
42	1	0	-2.681444	-1.401613	2.361336
43	1	0	-4.154390	-2.243625	2.813558
44	7	0	-4.848023	-2.805898	0.427687
45	1	0	-5.636666	-2.811284	1.057161
46	1	0	-4.930678	-3.352648	-0.415418
47	6	0	3.410340	3.802026	2.275972
48	6	0	1.430209	2.926041	3.566233
49	1	0	1.875723	0.119592	-3.584857
50	1	0	4.925974	0.315538	-3.148070
51	1	0	4.062923	0.852842	-4.611062
52	1	0	4.122996	-0.859868	-4.198057
53	1	0	2.082667	-3.842398	-1.335476
54	1	0	4.253187	-2.260986	0.156784
55	1	0	4.518512	-3.523311	-1.054773
56	1	0	3.776927	-3.956018	0.479291
57	1	0	-0.198594	-2.637301	2.295804
58	1	0	2.017553	-1.083968	3.761317
59	1	0	1.563242	-2.781462	4.063878
60	1	0	0.420605	-1.478040	4.419672
61	1	0	-0.330605	1.971480	1.811095
62	1	0	2.245841	2.398112	0.225122
63	1	0	1.161012	3.661515	0.816952
64	1	0	2.856644	1.743762	2.485563
65	1	0	-1.976555	1.994677	-2.273964
66	1	0	-3.742092	0.097614	-0.651062
67	1	0	-4.007173	0.446204	-2.360667
68	1	0	-1.260946	-0.583428	-1.523066
69	1	0	-2.105834	-0.800533	-3.052188
70	1	0	-3.749865	-2.319760	-1.808852
71	1	0	-2.088803	-2.934572	-1.889533
72	1	0	2.945183	4.789816	2.185877
73	1	0	4.032922	3.808391	3.173864
74	1	0	4.070303	3.657880	1.413724
75	1	0	0.822714	3.830004	3.438188
76	1	0	0.754876	2.079949	3.736941
77	1	0	2.023332	3.055645	4.475179

Rotational constants (GHZ): 0.1242034 0.0946259 0.0861679
ZPVE = 1780.0462 kJ mol^{-1}
E[M06-2X/6-31+G(d,p)] = -1713.95384694 a.u.
E[M06-2X/6-311++G(2d,p)] = -1714.40689556 a.u.

Table S13. M06-2X/6-31+G(d,p) Optimized Structure for z_2(LR) conformer rot-90flip

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.288227	0.715515	1.048881
2	6	0	0.954439	0.424394	0.565662
3	6	0	3.360281	-0.306508	1.062962
4	8	0	0.631162	-0.710546	0.144355
5	7	0	0.052389	1.444640	0.603672
6	6	0	-1.251193	1.381371	-0.031792
7	6	0	-1.476891	2.555818	-0.976915
8	8	0	-2.291579	2.537123	-1.859670
9	8	0	-0.718146	3.620644	-0.671413
10	6	0	-2.420706	1.371112	0.978529
11	6	0	-2.488679	0.164175	1.919808
12	6	0	-2.953780	-1.143024	1.272601
13	7	0	-1.876491	-1.701154	0.460558
14	6	0	-2.003485	-2.516212	-0.572041
15	7	0	-0.945805	-2.708742	-1.371158
16	7	0	-3.167819	-3.123899	-0.839311
17	6	0	4.420570	-0.078241	-0.045223
18	1	0	0.376007	2.359930	0.892278
19	1	0	-0.941840	4.345595	-1.278007
20	1	0	-0.094189	-2.186176	-1.184656
21	1	0	-0.914687	-3.475791	-2.023962
22	1	0	-3.926582	-3.103234	-0.176148
23	1	0	-3.301440	-3.646798	-1.690856
24	1	0	-0.924059	-1.327810	0.589286
25	6	0	5.544992	-1.101608	0.105602
26	6	0	3.786400	-0.159048	-1.433585
27	1	0	2.512465	1.731943	1.362815
28	1	0	3.867887	-0.278867	2.035816
29	1	0	2.919427	-1.300798	0.934073
30	1	0	-1.273541	0.487966	-0.659353
31	1	0	-3.353742	1.450469	0.408828
32	1	0	-2.340387	2.281035	1.584824
33	1	0	-1.520219	0.003584	2.411985
34	1	0	-3.197879	0.399468	2.718482
35	1	0	-3.826782	-0.951775	0.635452
36	1	0	-3.241047	-1.859203	2.051202
37	1	0	4.841605	0.926998	0.092160
38	1	0	5.156890	-2.119261	-0.017513
39	1	0	6.316753	-0.943950	-0.652862
40	1	0	6.019313	-1.035801	1.089242
41	1	0	3.321541	-1.140981	-1.582053
42	1	0	3.014784	0.604961	-1.577837
43	1	0	4.541249	-0.021641	-2.212640

Rotational constants (GHZ): 0.3991937 0.2281453 0.1758241
ZPVE = 989.8109 kJ mol^{-1}
E[M06-2X/6-31+G(d,p)] = -915.8884626 a.u.
E[M06-2X/6-311++G(2d,p)] = -916.1299738 a.u.

Table S14. B3LYP/6-31+G(d,p) Optimized Structure for $\mathbf{z_2}$(LR) conformer rot-90flip

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.263558	0.516918	0.855628
2	6	0	0.895064	0.370227	0.409824
3	6	0	3.257484	-0.583490	0.825213
4	8	0	0.448838	-0.706402	-0.072468
5	7	0	0.085703	1.465900	0.552202
6	6	0	-1.243019	1.576161	-0.038707
7	6	0	-1.407089	2.870631	-0.840514
8	8	0	-2.262929	3.020250	-1.679369
9	8	0	-0.532433	3.833048	-0.472439
10	6	0	-2.397089	1.507277	1.001101
11	6	0	-2.550064	0.194944	1.791099
12	6	0	-3.104309	-1.013254	1.017826
13	7	0	-2.074372	-1.605448	0.158808
14	6	0	-2.191479	-2.714951	-0.555682
15	7	0	-1.099303	-3.202642	-1.176272
16	7	0	-3.363743	-3.367451	-0.663221
17	6	0	4.600472	-0.209040	0.135644
18	1	0	0.504255	2.323664	0.889797
19	1	0	-0.717991	4.633025	-0.995851
20	1	0	-0.227036	-2.691095	-1.104323
21	1	0	-1.172420	-3.917803	-1.883098
22	1	0	-4.201027	-3.008418	-0.232519
23	1	0	-3.427403	-4.261062	-1.126220
24	1	0	-1.127042	-1.174314	0.144135
25	6	0	5.628170	-1.330204	0.340723
26	6	0	4.399465	0.099081	-1.355164
27	1	0	2.570370	1.486091	1.245915
28	1	0	3.486387	-0.863916	1.867502
29	1	0	2.818715	-1.466299	0.348339
30	1	0	-1.347407	0.771459	-0.769080
31	1	0	-3.330119	1.725656	0.469463
32	1	0	-2.246859	2.320228	1.721074
33	1	0	-1.605399	-0.083021	2.274094
34	1	0	-3.255392	0.391176	2.605299
35	1	0	-3.965069	-0.699349	0.411000
36	1	0	-3.450152	-1.766534	1.737099
37	1	0	4.983414	0.697306	0.626784
38	1	0	5.288323	-2.265203	-0.121323
39	1	0	6.586887	-1.065058	-0.116247
40	1	0	5.807199	-1.524946	1.403635
41	1	0	4.014293	-0.779362	-1.887677
42	1	0	3.693468	0.922679	-1.511902
43	1	0	5.347215	0.381618	-1.824261

Rotational constants (GHZ): 0.3628329 0.2196108 0.1572548

ZPVE = 978.6642 kJ mol^{-1}
E[B3LYP/6-31+G(d,p)] = -916.3061046 a.u.
E[B3LYP/6-311++G(2d,p)] = -916.5280014 a.u.
E[PMP2/6-311++G(2d,p)] = -914.0998288 a.u.

Table S15. M06-2X/6-31+G(d,p) Optimized Structure for z_2(LR) conformer 1-2flip120

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.214594	-1.446954	-0.423308
2	6	0	-0.893192	-0.854887	-0.395875
3	6	0	-3.405560	-0.676323	-0.849038
4	8	0	-0.675596	0.305673	-0.814957
5	7	0	0.106378	-1.611489	0.135826
6	6	0	1.508350	-1.240980	0.077326
7	6	0	2.361830	-2.356064	-0.515453
8	8	0	3.446800	-2.165804	-0.995412
9	8	0	1.797587	-3.566506	-0.378310
10	6	0	2.101049	-0.893707	1.461924
11	6	0	1.502990	0.328067	2.167297
12	6	0	1.909559	1.683352	1.581784
13	7	0	1.180142	1.921350	0.339514
14	6	0	1.575153	2.663619	-0.681059
15	7	0	0.942939	2.530627	-1.853952
16	7	0	2.602138	3.516854	-0.563698
17	6	0	-4.256070	-0.194119	0.355895
18	1	0	-0.104048	-2.565345	0.403974
19	1	0	2.406121	-4.235874	-0.732343
20	1	0	0.220395	1.820621	-1.938831
21	1	0	1.042823	3.217478	-2.584617
22	1	0	2.987510	3.742934	0.339863
23	1	0	2.981862	3.990865	-1.368425
24	1	0	0.358005	1.333716	0.139718
25	6	0	-3.447178	0.736266	1.260315
26	6	0	-5.520086	0.496896	-0.152105
27	1	0	-2.335069	-2.460295	-0.049068
28	1	0	-3.089527	0.196495	-1.430653
29	1	0	-4.035931	-1.307039	-1.487296
30	1	0	1.602784	-0.396676	-0.608905
31	1	0	3.181535	-0.757511	1.337165
32	1	0	1.963415	-1.769232	2.107329
33	1	0	0.407062	0.258381	2.199258
34	1	0	1.836478	0.311721	3.208760
35	1	0	2.987365	1.689872	1.375682
36	1	0	1.687706	2.479696	2.301275
37	1	0	-4.550347	-1.079367	0.935874
38	1	0	-3.110481	1.616018	0.699113
39	1	0	-4.054408	1.082213	2.101457
40	1	0	-2.561928	0.237007	1.671461
41	1	0	-5.263689	1.387600	-0.736958
42	1	0	-6.112704	-0.167121	-0.788033
43	1	0	-6.149940	0.814545	0.683587

Rotational constants (GHZ): 0.3923142 0.2410369 0.1807311

ZPVE = 991.0723 kJ mol^{-1}

E[M06-2X/6-31+G(d,p)] = -915.8888626 a.u.

E[M06-2X/6-311++G(2d,p)] = -916.1302472 a.u.

Table S16. B3LYP/6-31+G(d,p) Optimized Structure for $\mathbf{z_2}$(LR) conformer 1-2flip120

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.264595	-1.015360	-0.301929
2	6	0	-0.867695	-0.639534	-0.305439
3	6	0	-3.356734	-0.110938	-0.737479
4	8	0	-0.470518	0.496311	-0.683428
5	7	0	0.019045	-1.584047	0.139011
6	6	0	1.465567	-1.476379	-0.012719
7	6	0	2.067407	-2.732398	-0.649979
8	8	0	3.150809	-2.744347	-1.183519
9	8	0	1.284195	-3.824137	-0.503762
10	6	0	2.217091	-1.210469	1.322088
11	6	0	1.924113	0.120303	2.039107
12	6	0	2.497836	1.391853	1.391869
13	7	0	1.707458	1.787227	0.222489
14	6	0	1.905767	2.855934	-0.535121
15	7	0	1.014689	3.134685	-1.506465
16	7	0	2.962534	3.668458	-0.349036
17	6	0	-4.584242	-0.095143	0.214353
18	1	0	-0.343648	-2.499011	0.376176
19	1	0	1.742575	-4.586676	-0.899708
20	1	0	0.239105	2.499599	-1.657505
21	1	0	1.208192	3.824702	-2.215466
22	1	0	3.649336	3.473440	0.361962
23	1	0	3.066154	4.524675	-0.871540
24	1	0	0.871288	1.220990	-0.029286
25	6	0	-4.215074	0.463232	1.596528
26	6	0	-5.734780	0.698625	-0.419060
27	1	0	-2.519242	-2.024874	0.017168
28	1	0	-2.965221	0.902742	-0.876969
29	1	0	-3.704851	-0.450815	-1.728471
30	1	0	1.665202	-0.671212	-0.722302
31	1	0	3.290371	-1.284721	1.113678
32	1	0	1.972417	-2.027231	2.011108
33	1	0	0.847046	0.248328	2.202512
34	1	0	2.370651	0.052061	3.036584
35	1	0	3.541931	1.216389	1.097367
36	1	0	2.483024	2.204074	2.129952
37	1	0	-4.918337	-1.135271	0.340900
38	1	0	-3.871926	1.502491	1.519240
39	1	0	-5.080936	0.449416	2.266092
40	1	0	-3.418192	-0.119623	2.073073
41	1	0	-5.449569	1.745698	-0.578722
42	1	0	-6.029948	0.278494	-1.386578
43	1	0	-6.615361	0.691093	0.231106

Rotational constants (GHZ): 0.3562551 0.2211675 0.1593516

ZPVE = 978.4908 kJ mol^{-1}

E[B3LYP/6-31+G(d,p)] = -916.3061115 a.u.

E[B3LYP/6-311++G(2d,p)] = -916.5279604 a.u.

E[PMP2/6-311++G(2d,p)] = -914.0997619 a.u.

E[CCSD(T)/6-31G(d)] = -913.5697647 a.u.

E[PMP2/6-31G(d)] = -913.33729856 a.u.

E[PMP2/aug-cc-pVTZ] = -914.5577366 a.u.

E[CCSD(T)/6-311+G(2d,p)] = -914.3322949 a.u.

E[CCSD(T)/aug-cc-pVTZ] = -914.7902027 a.u.

Table S17. M06-2X/6-31+G(d,p) Optimized Structure for w_2(LR) fragment ion.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.369283	-2.511479	-0.219412
2	6	0	1.318526	-1.462825	-0.272070
3	6	0	3.435837	-2.479918	0.579061
4	8	0	0.167867	-1.755186	-0.641782
5	7	0	1.652480	-0.209551	0.103954
6	6	0	0.751236	0.924974	-0.017354
7	6	0	1.411139	2.086340	-0.751729
8	8	0	0.784701	2.978307	-1.256704
9	8	0	2.751595	2.030214	-0.712314
10	6	0	0.258265	1.459777	1.345364
11	6	0	-0.611356	0.508659	2.174270
12	6	0	-2.041211	0.315580	1.660345
13	7	0	-2.033284	-0.561666	0.491924
14	6	0	-2.891034	-0.554613	-0.515628
15	7	0	-2.564445	-1.199695	-1.642111
16	7	0	-4.054769	0.103653	-0.430848
17	1	0	2.632885	0.000688	0.246885
18	1	0	3.109901	2.814724	-1.159433
19	1	0	-1.641758	-1.619252	-1.714912
20	1	0	-3.259848	-1.429409	-2.334708
21	1	0	-4.387927	0.457220	0.452519
22	1	0	-4.646513	0.223364	-1.238514
23	1	0	-1.200480	-1.138332	0.332832
24	1	0	2.159378	-3.365403	-0.855818
25	1	0	3.632412	-1.662702	1.268584
26	1	0	4.144470	-3.300830	0.588430
27	1	0	-0.091435	0.618687	-0.641281
28	1	0	-0.289117	2.390269	1.155911
29	1	0	1.143061	1.726467	1.934868
30	1	0	-0.125281	-0.470620	2.280506
31	1	0	-0.685493	0.917899	3.185819
32	1	0	-2.468665	1.285927	1.378590
33	1	0	-2.662883	-0.123526	2.448611

Rotational constants (GHZ): 0.5886643 0.3762057 0.2982578

ZPVE = 740.6577 kJ mol^{-1}

E[M06-2X/6-31+G(d,p)] = -797.423063481 a.u.

E[M06-2X/6-311++G(2d,p)] = -797.638160472 a.u.

Table S18. B3LYP/6-31+G(d,p) Optimized Structure for w_2(LR) fragment ion.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.989932	2.786537	0.340312
2	6	0	-1.141036	1.599813	0.085756
3	6	0	-1.514913	4.028869	0.199747
4	8	0	0.046208	1.691049	-0.301802
5	7	0	-1.728485	0.397449	0.311644
6	6	0	-1.132499	-0.886668	-0.047460
7	6	0	-2.111431	-1.766606	-0.829564
8	8	0	-1.754956	-2.689025	-1.522382
9	8	0	-3.402993	-1.432838	-0.615918

10	6	0	-0.623914	-1.702177	1.173654
11	6	0	0.532174	-1.097549	1.991402
12	6	0	1.920967	-1.109420	1.331886
13	7	0	2.023892	-0.060450	0.312130
14	6	0	3.034800	0.132876	-0.523400
15	7	0	2.919470	1.085275	-1.468854
16	7	0	4.157100	-0.606082	-0.457609
17	1	0	-2.705941	0.387116	0.576271
18	1	0	-3.968185	-2.050260	-1.113767
19	1	0	2.074089	1.643018	-1.504837
20	1	0	3.715980	1.395996	-2.003198
21	1	0	4.282125	-1.300962	0.261474
22	1	0	4.877155	-0.531977	-1.159971
23	1	0	1.232088	0.599635	0.201943
24	1	0	-3.019755	2.613588	0.643469
25	1	0	-0.486616	4.199955	-0.102959
26	1	0	-2.142259	4.894906	0.381283
27	1	0	-0.309927	-0.686032	-0.735904
28	1	0	-0.331547	-2.691917	0.805282
29	1	0	-1.472761	-1.856670	1.849948
30	1	0	0.291817	-0.077740	2.316338
31	1	0	0.619397	-1.687818	2.909407
32	1	0	2.108395	-2.090359	0.874736
33	1	0	2.680729	-0.941354	2.106120

Rotational constants (GHZ): 0.5377247 0.3758226 0.2718081

ZPVE = 731.4957 kJ mol^{-1}

E[B3LYP/6-31+G(d,p)] = -797.771055962 a.u.

E[B3LYP/6-311++G(2d,p)] = -797.970349261 a.u.

E[MP2/6-311++G(2d,p)] = -795.9191469 a.u.

E[CCSD(T)/6-31G(d)] = -795.4582697 a.u.

E[MP2/6-31G(d)] = -795.27482409936 a.u.

E[MP2/aug-cc-pVTZ] = -796.306219 a.u.

E[CCSD(T)/6-311+G(2d,p)] = -796.1025925 a.u.

E[CCSD(T)/aug-cc-pVTZ] = -796.4896646 a.u.

Table S19. B3LYP/6-31+G(d,p) Optimized Structure for TS $\mathbf{z_2}$(LR) → $\mathbf{w_2}$(LR)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.959951	-1.807587	-0.585975
2	6	0	-0.726720	-1.037100	-0.448352
3	6	0	-3.090626	-1.270013	-1.115364
4	8	0	-0.618259	0.160073	-0.826234
5	7	0	0.330192	-1.689265	0.121150
6	6	0	1.704079	-1.200635	0.090991
7	6	0	2.673441	-2.250061	-0.460575
8	8	0	3.763752	-1.971957	-0.900822
9	8	0	2.201934	-3.512074	-0.354194
10	6	0	2.236201	-0.738076	1.476002
11	6	0	1.535902	0.470377	2.123138
12	6	0	1.802323	1.841877	1.481196
13	7	0	1.054479	1.982145	0.228084
14	6	0	1.211537	2.925804	-0.688256
15	7	0	0.552220	2.804715	-1.857036
16	7	0	2.017478	3.985324	-0.486055
17	6	0	-4.610910	-0.355117	0.622589
18	1	0	0.206363	-2.667151	0.351778
19	1	0	2.880491	-4.122658	-0.693234

20	1	0	-0.046098	1.996985	-1.996601
21	1	0	0.464308	3.581849	-2.493166
22	1	0	2.491702	4.117207	0.393270
23	1	0	2.245051	4.620848	-1.235343
24	1	0	0.372650	1.239179	-0.030580
25	6	0	-3.702690	0.400889	1.535556
26	6	0	-5.593546	0.373802	-0.235567
27	1	0	-1.946814	-2.842417	-0.253126
28	1	0	-3.074455	-0.269637	-1.533111
29	1	0	-3.939814	-1.899452	-1.351748
30	1	0	1.745381	-0.373536	-0.619446
31	1	0	3.305084	-0.524296	1.363073
32	1	0	2.155652	-1.585949	2.166293
33	1	0	0.453770	0.303087	2.188666
34	1	0	1.890564	0.536126	3.157017
35	1	0	2.876828	1.960198	1.286357
36	1	0	1.494187	2.628110	2.182532
37	1	0	-4.887494	-1.359878	0.938027
38	1	0	-3.261125	1.272285	1.038237
39	1	0	-4.259598	0.777481	2.409946
40	1	0	-2.896146	-0.232090	1.919982
41	1	0	-5.136499	1.232994	-0.741041
42	1	0	-6.048704	-0.275524	-0.990264
43	1	0	-6.419513	0.772520	0.377185

Rotational constants (GHZ): 0.3573376 0.2328126 0.1700458

ZPVE = 968.2471 kJ mol^{-1}
E[B3LYP/6-31+G(d,p)] = -916.26409221 a.u.
E[B3LYP/6-311++G(2d,p)] = -916.487368128 a.u.
E[PMP2/6-311++G(2d,p)] = -914.050878 a.u.
E[CCSD(T)/6-31G(d)] = -913.5191589 a.u.
E[PMP2/6-31G(d)] = -913.284395 a.u.
E[PMP2/aug-cc-pVTZ] = -914.5056781 a.u.
E[CCSD(T)/6-311+G(2d,p)] = -914.2856419a.u.
E[CCSD(T)/aug-cc-pVTZ] = -914.740442 a.u.

Table S20. M06-2X/6-31+G(d,p) Optimized Structure for TS $\mathbf{z_2}$(LR) → $\mathbf{w_2}$(LR)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.007518	-1.882252	-0.637729
2	6	0	-0.790016	-1.080191	-0.531954
3	6	0	-3.133134	-1.337159	-1.154067
4	8	0	-0.714496	0.093288	-0.962969
5	7	0	0.268958	-1.667148	0.082705
6	6	0	1.595266	-1.082995	0.134864
7	6	0	2.663469	-2.051716	-0.357685
8	8	0	3.745272	-1.692642	-0.739270
9	8	0	2.287030	-3.335620	-0.253993
10	6	0	2.000627	-0.631594	1.556328
11	6	0	1.147816	0.480077	2.176488
12	6	0	1.390665	1.879758	1.605038
13	7	0	0.785485	1.984213	0.279166
14	6	0	1.248838	2.673938	-0.750218
15	7	0	0.792317	2.382359	-1.974278
16	7	0	2.173468	3.631330	-0.587727
17	6	0	-4.351758	-0.234923	0.621630
18	1	0	0.182830	-2.637508	0.359359
19	1	0	3.023485	-3.899654	-0.542070

20	1	0	0.166793	1.587404	-2.083132
21	1	0	0.936095	3.006885	-2.751868
22	1	0	2.404129	3.977329	0.330316
23	1	0	2.621751	4.064365	-1.380188
24	1	0	0.062128	1.293253	0.026621
25	6	0	-3.232154	0.375198	1.395956
26	6	0	-5.260244	0.638478	-0.177051
27	1	0	-1.990006	-2.900009	-0.259185
28	1	0	-3.090037	-0.351250	-1.607603
29	1	0	-4.016693	-1.940097	-1.332046
30	1	0	1.617684	-0.241262	-0.560018
31	1	0	3.050767	-0.318978	1.522415
32	1	0	1.952662	-1.512302	2.207430
33	1	0	0.079510	0.234689	2.099295
34	1	0	1.372137	0.523509	3.246211
35	1	0	2.469152	2.063829	1.524824
36	1	0	0.958131	2.634906	2.270410
37	1	0	-4.768956	-1.160208	1.011738
38	1	0	-2.684909	1.102850	0.784440
39	1	0	-3.610580	0.905225	2.282511
40	1	0	-2.529612	-0.388249	1.747577
41	1	0	-4.695882	1.378342	-0.755723
42	1	0	-5.887207	0.061443	-0.862653
43	1	0	-5.938561	1.200284	0.482528

Rotational constants (GHZ): 0.3910635 0.2497770 0.1893850

ZPVE = 978.8039 kJ mol^{-1}

E[M06-2X/6-31+G(d,p)] = -915.840052746 a.u.

E[M06-2X/6-311++G(2d,p)] = -916.082589009 a.u.

Table S21. M06-2X/6-31+G(d,p) Optimized Structure for $\mathbf{z_2}$(LK) conformer rot90flip120

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.071956	2.219948	0.290455
2	6	0	1.791020	-0.653107	-1.081643
3	6	0	3.059090	0.088349	-0.892960
4	6	0	0.555037	-0.263089	-0.438793
5	8	0	0.465681	0.762673	0.286424
6	6	0	-2.317585	-2.310472	0.307003
7	8	0	-1.869551	-3.301835	-0.211899
8	8	0	-3.366734	-2.293593	1.129972
9	1	0	-3.697119	-3.201223	1.234706
10	7	0	-0.516144	-1.060871	-0.640734
11	1	0	-0.391384	-1.950242	-1.115980
12	6	0	-1.773598	-0.909153	0.066200
13	6	0	-2.811433	-0.086528	-0.724641
14	6	0	-2.380825	1.362304	-0.952203
15	6	0	-2.491542	2.229083	0.309332
16	6	0	-1.664261	3.506459	0.215609
17	7	0	-0.232533	3.213706	0.584556
18	1	0	0.415598	3.903314	0.200973
19	1	0	-0.118346	3.223860	1.600969
20	6	0	4.068609	-0.677333	0.001967
21	6	0	5.388527	0.089242	0.057028
22	6	0	3.498460	-0.895899	1.403029
23	1	0	1.790753	-1.561906	-1.677699
24	1	0	3.525422	0.256777	-1.872346
25	1	0	2.855563	1.064056	-0.437534
26	1	0	-1.572879	-0.443225	1.037329

27	1	0	-3.763011	-0.118326	-0.182324
28	1	0	-2.968663	-0.581029	-1.689433
29	1	0	-1.357062	1.373257	-1.346301
30	1	0	-3.010870	1.802303	-1.732515
31	1	0	-2.181205	1.671221	1.202814
32	1	0	-3.537734	2.504534	0.472971
33	1	0	-1.660887	3.899968	-0.803584
34	1	0	-2.020368	4.289694	0.886624
35	1	0	4.251105	-1.656049	-0.461850
36	1	0	5.242261	1.076057	0.511598
37	1	0	5.813417	0.233674	-0.940682
38	1	0	6.122917	-0.450016	0.661595
39	1	0	3.263452	0.065805	1.874735
40	1	0	4.221813	-1.414354	2.038213
41	1	0	2.581832	-1.495043	1.384976

Rotational constants (GHZ): 0.5078616 0.2721631 0.1962002

ZPVE = 964.8015 kJ mol^{-1}

E[M06-2X/6-31+G(d,p)] = -806.3857069 a.u.

E[M06-2X/6-311++G(2d,p)] = -806.597372 a.u.

Table S22. B3LYP/6-31+G(d,p) Optimized Structure for z_2(LK) conformer rot90flip120

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.433715	2.224345	0.543392
2	6	0	1.903632	-0.424416	-0.829222
3	6	0	3.093241	0.436492	-0.622507
4	6	0	0.590626	-0.120245	-0.304826
5	8	0	0.359653	0.918972	0.378390
6	6	0	-2.087549	-2.472496	0.299425
7	8	0	-1.501810	-3.420360	-0.176702
8	8	0	-3.152809	-2.567188	1.110884
9	1	0	-3.365559	-3.509688	1.234773
10	7	0	-0.394412	-1.017928	-0.584214
11	1	0	-0.136223	-1.896609	-1.024336
12	6	0	-1.720047	-1.014467	0.019517
13	6	0	-2.800383	-0.362866	-0.885665
14	6	0	-2.605970	1.147603	-1.085731
15	6	0	-3.028020	2.000405	0.132501
16	6	0	-2.280935	3.331493	0.233667
17	7	0	-0.919110	3.127805	0.868055
18	1	0	-0.293658	3.917052	0.690458
19	1	0	-1.006904	3.038806	1.883557
20	6	0	4.360487	-0.336351	-0.158752
21	6	0	5.578416	0.597237	-0.166016
22	6	0	4.153159	-0.975602	1.221947
23	1	0	2.015959	-1.335389	-1.414609
24	1	0	3.334134	0.923148	-1.583690
25	1	0	2.855855	1.236830	0.086950
26	1	0	-1.662718	-0.486752	0.977313
27	1	0	-3.785460	-0.561702	-0.449322
28	1	0	-2.772850	-0.867144	-1.857773
29	1	0	-1.559652	1.338127	-1.349771
30	1	0	-3.194355	1.465886	-1.953251
31	1	0	-2.894987	1.448102	1.072665
32	1	0	-4.099167	2.219572	0.074342
33	1	0	-2.108840	3.769440	-0.752684
34	1	0	-2.812986	4.063246	0.845472
35	1	0	4.542043	-1.139308	-0.887667

36	1	0	5.441409	1.427805	0.537332
37	1	0	5.756856	1.021787	-1.159951
38	1	0	6.482078	0.056993	0.133208
39	1	0	3.956141	-0.209954	1.982564
40	1	0	5.045668	-1.528368	1.531482
41	1	0	3.311374	-1.677488	1.226049

Rotational constants (GHZ): 0.5077382 0.2478178 0.1822019

ZPVE = 955.9999 kJ mol^{-1}

E[B3LYP/6-31+G(d,p)] = -806.7656224 a.u.

E[B3LYP/6-311++G(2d,p)] = -806.9585881 a.u.

E[PMP2/6-311++G(2d,p)] = -804.7863695a.u.

Table S23. M06-2X/6-31+G(d,p) Optimized Structure for z_2(LK) conformer 4-2flip

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.881553	1.569313	-0.780147
2	6	0	-1.354022	-1.829876	-0.021491
3	6	0	-2.723721	-1.622126	-0.549384
4	6	0	-0.272430	-0.909534	-0.300373
5	8	0	-0.437088	0.138827	-0.978667
6	6	0	3.294282	-1.430333	-0.152215
7	8	0	3.218601	-2.577563	0.210062
8	8	0	4.402346	-0.853735	-0.618510
9	1	0	5.120283	-1.508375	-0.615935
10	7	0	0.941659	-1.216445	0.201531
11	1	0	1.097981	-2.128346	0.621606
12	6	0	2.136056	-0.445808	-0.087320
13	6	0	2.431058	0.618193	0.990771
14	6	0	1.326404	1.666331	1.126195
15	6	0	1.303777	2.682793	-0.022639
16	6	0	-0.021424	3.434711	-0.107667
17	7	0	-1.018334	2.634567	-0.905659
18	1	0	-1.982180	2.889498	-0.685035
19	1	0	-0.881058	2.792760	-1.906887
20	6	0	-3.693724	-1.009725	0.494223
21	6	0	-3.276133	0.414915	0.861997
22	6	0	-5.120343	-1.030773	-0.052061
23	1	0	-1.146841	-2.685294	0.615692
24	1	0	-2.685751	-0.965198	-1.426232
25	1	0	-3.128962	-2.589457	-0.868510
26	1	0	2.018071	0.023214	-1.070033
27	1	0	3.384699	1.099740	0.746921
28	1	0	2.562883	0.100333	1.947276
29	1	0	0.357194	1.158589	1.215260
30	1	0	1.468692	2.208869	2.067079
31	1	0	1.498267	2.194867	-0.986564
32	1	0	2.106967	3.412067	0.118956
33	1	0	-0.452223	3.585707	0.885028
34	1	0	0.076804	4.407653	-0.591585
35	1	0	-3.654597	-1.628285	1.400371
36	1	0	-3.336011	1.049174	-0.033397
37	1	0	-2.253588	0.455210	1.257400
38	1	0	-3.946562	0.836579	1.615867
39	1	0	-5.187869	-0.443267	-0.975145
40	1	0	-5.821606	-0.605052	0.670957
41	1	0	-5.445886	-2.049974	-0.277329

Rotational constants (GHZ): 0.5937316 0.2733364 0.2034671

ZPVE = 966.3673 kJ mol^{-1}
E[M06-2X/6-31+G(d,p)] = -806.387251 a.u.
E[M06-2X/6-311++G(2d,p)] = -806.5989288 a.u.

Table S24. B3LYP/6-31+G(d,p) Optimized Structure for $\mathbf{z_2}$(LK) conformer 4-2flip

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.085476	1.997206	-0.911676
2	6	0	-1.800917	-1.242796	-0.201157
3	6	0	-3.080060	-0.710848	-0.729481
4	6	0	-0.530111	-0.566260	-0.341087
5	8	0	-0.422642	0.549462	-0.926751
6	6	0	2.744294	-2.094835	-0.203133
7	8	0	2.334109	-3.196218	0.091136
8	8	0	3.966698	-1.846661	-0.699795
9	1	0	4.450342	-2.689419	-0.769137
10	7	0	0.551883	-1.198885	0.191279
11	1	0	0.432944	-2.146138	0.539100
12	6	0	1.938723	-0.807482	-0.020441
13	6	0	2.524346	0.018804	1.156791
14	6	0	1.899943	1.415694	1.294700
15	6	0	2.418370	2.436378	0.254944
16	6	0	1.403521	3.525291	-0.095697
17	7	0	0.401488	3.007582	-1.107720
18	1	0	-0.429490	3.601398	-1.159288
19	1	0	0.814166	2.990366	-2.043853
20	6	0	-4.229192	-0.664541	0.319000
21	6	0	-3.909679	0.312191	1.459926
22	6	0	-5.554772	-0.308157	-0.366960
23	1	0	-1.807834	-2.205391	0.307412
24	1	0	-2.920255	0.281791	-1.163807
25	1	0	-3.407514	-1.368776	-1.551821
26	1	0	1.998839	-0.232834	-0.950480
27	1	0	3.608025	0.102739	1.019003
28	1	0	2.361854	-0.549214	2.079185
29	1	0	0.809376	1.323455	1.239231
30	1	0	2.115396	1.800311	2.297348
31	1	0	2.734353	1.937579	-0.671678
32	1	0	3.318506	2.927144	0.639053
33	1	0	0.833568	3.839871	0.782162
34	1	0	1.874171	4.408352	-0.533504
35	1	0	-4.327212	-1.672464	0.746870
36	1	0	-3.800686	1.335540	1.078253
37	1	0	-2.983235	0.044082	1.981035
38	1	0	-4.715139	0.321046	2.200923
39	1	0	-5.505801	0.686256	-0.827500
40	1	0	-6.375408	-0.297473	0.357398
41	1	0	-5.810156	-1.029605	-1.150296

Rotational constants (GHZ): 0.5238474 0.2477818 0.1872131

ZPVE = 955.9867 kJ mol^{-1}
E[B3LYP/6-31+G(d,p)] = -806.7655225 a.u.
E[B3LYP/6-311++G(2d,p)] = -806.9584335 a.u.
E[PMP2/6-311++G(2d,p)] = -804.7863695 a.u.
E[CCSD(T)/6-31G(d)] = -804.316195 a.u.
E[PMP2/6-31G(d)] = -804.096348 a.u.
E[PMP2/aug-cc-pVTZ] = -805.191520 a.u.
E[CCSD(T)/6-311+G(2d,p)] = -805.411367 a.u.
E[CCSD(T)/aug-cc-pVTZ] = -805.006217 a.u.

Table S25. B3LYP/6-31+G(d,p) Optimized Structure for w_2(LK) fragment ion

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.252627	0.963082	-0.725664
2	6	0	-0.836225	3.037671	-0.127282
3	6	0	-1.751576	3.439957	0.762169
4	6	0	-0.352163	1.646535	-0.307611
5	8	0	0.763837	1.447025	-0.848579
6	6	0	-2.190812	-1.467782	-0.355849
7	8	0	-3.261408	-0.954309	-0.113036
8	8	0	-2.034746	-2.708655	-0.840777
9	1	0	-2.914404	-3.112066	-0.952554
10	7	0	-1.132318	0.631588	0.110045
11	1	0	-2.095154	0.827571	0.368828
12	6	0	-0.845232	-0.782278	-0.115193
13	6	0	-0.111146	-1.457202	1.073823
14	6	0	1.316452	-0.938153	1.305232
15	6	0	2.349377	-1.460129	0.281095
16	6	0	3.562646	-0.542719	0.113388
17	7	0	3.245206	0.591010	-0.844844
18	1	0	3.903312	1.368248	-0.750249
19	1	0	3.299889	0.267545	-1.814224
20	1	0	-0.330489	3.752036	-0.770006
21	1	0	-2.245718	2.764321	1.455525
22	1	0	-2.025274	4.487196	0.838491
23	1	0	-0.248897	-0.872598	-1.029105
24	1	0	-0.093046	-2.538292	0.897301
25	1	0	-0.708806	-1.290973	1.976818
26	1	0	1.300212	0.157169	1.318535
27	1	0	1.638940	-1.242368	2.307188
28	1	0	1.890554	-1.623325	-0.703369
29	1	0	2.714207	-2.442821	0.597600
30	1	0	3.852462	-0.083390	1.061662
31	1	0	4.429989	-1.067408	-0.292678

Rotational constants (GHZ): 0.6860326 0.5207855 0.3363922

ZPVE = 708.2938 kJ mol^{-1}

E[B3LYP/6-31+G(d,p)] = -688.2275623 a.u.

E[B3LYP/6-311++G(2d,p)] = -688.3981218 a.u.

E[MP2/6-311++G(2d,p)] = -686.6036471 a.u.

E[CCSD(T)/6-31G(d)] = -686.2033222 a.u.

E[MP2/6-31G(d)] = -686.03337475512 a.u.

E[MP2/aug-cc-pVTZ] = -686.9403859 a.u.

E[CCSD(T)/6-311+G(2d,p)] = -686.773595 a.u.

E[CCSD(T)/aug-cc-pVTZ] = -687.110333 a.u.

Table S26. M06-2X/6-31+G(d,p) Optimized Structure for w_2(LK) fragment ion

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.443110	0.673932	-0.635716
2	6	0	-0.189088	3.059338	-0.163489
3	6	0	-0.897685	3.611468	0.821773
4	6	0	-0.042555	1.596590	-0.365290
5	8	0	0.979075	1.132861	-0.916197

6	6	0	-2.475042	-1.065354	-0.319233
7	8	0	-3.411576	-0.343494	-0.085174
8	8	0	-2.573799	-2.333316	-0.717750
9	1	0	-3.513878	-2.568983	-0.787565
10	7	0	-1.027906	0.794864	0.055862
11	1	0	-1.924528	1.195965	0.317214
12	6	0	-1.022173	-0.643143	-0.154485
13	6	0	-0.390586	-1.420788	1.017701
14	6	0	1.090030	-1.106067	1.238540
15	6	0	2.006088	-1.723589	0.172955
16	6	0	3.392944	-1.087009	0.147217
17	7	0	3.373844	0.156832	-0.706994
18	1	0	4.144315	0.790687	-0.487416
19	1	0	3.454582	-0.090253	-1.696662
20	1	0	0.384474	3.661415	-0.861368
21	1	0	-1.435727	3.019947	1.558220
22	1	0	-0.943754	4.689032	0.935613
23	1	0	-0.491583	-0.855064	-1.089471
24	1	0	-0.523567	-2.491670	0.827298
25	1	0	-0.955505	-1.179747	1.924924
26	1	0	1.226571	-0.018891	1.290231
27	1	0	1.388440	-1.494145	2.218390
28	1	0	1.560535	-1.643606	-0.827134
29	1	0	2.122796	-2.793614	0.369360
30	1	0	3.707707	-0.783590	1.148422
31	1	0	4.153241	-1.750372	-0.267587

Rotational constants (GHZ): 0.7237890 0.5197552 0.3411294

ZPVE = 714.8678 kJ mol^{-1}

E[M06-2X/6-31+G(d,p)] = -687.9175643 a.u.

E[M06-2X/6-311++G(2d,p)] = -688.1031291 a.u.

Table S27. M06-2X/6-31+G(d,p) Optimized Structure for TS $\mathbf{z_2}$(LK) → $\mathbf{w_2}$(LK)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.081276	2.248491	-0.165412
2	6	0	-1.693907	-0.398911	1.561781
3	6	0	-2.836305	0.308144	1.425920
4	6	0	-0.548198	-0.138455	0.691820
5	8	0	-0.512960	0.820485	-0.125005
6	6	0	2.092818	-2.373361	-0.310725
7	8	0	1.674029	-3.314851	0.314480
8	8	0	3.022521	-2.450414	-1.264625
9	1	0	3.295523	-3.377706	-1.361571
10	7	0	0.493859	-0.981886	0.793648
11	1	0	0.399445	-1.822320	1.356307
12	6	0	1.653709	-0.935988	-0.075317
13	6	0	2.822266	-0.136464	0.536515
14	6	0	2.482381	1.335777	0.767463
15	6	0	2.449250	2.159542	-0.526536
16	6	0	1.699386	3.476145	-0.355094
17	7	0	0.216858	3.240954	-0.495089
18	1	0	-0.334408	3.950096	-0.009676
19	1	0	-0.054642	3.269190	-1.480565
20	6	0	-4.241076	-0.798138	-0.290946
21	6	0	-5.093246	0.353839	-0.706431
22	6	0	-3.177956	-1.303237	-1.205270
23	1	0	-1.615718	-1.214632	2.274339
24	1	0	-3.665853	0.170325	2.110023

25	1	0	-2.876717	1.152900	0.744767
26	1	0	1.350780	-0.502572	-1.034743
27	1	0	3.689471	-0.227048	-0.127146
28	1	0	3.089874	-0.606386	1.489428
29	1	0	1.523762	1.403539	1.297668
30	1	0	3.229598	1.772300	1.438752
31	1	0	1.987155	1.592983	-1.345664
32	1	0	3.471865	2.381120	-0.846437
33	1	0	1.867400	3.897525	0.638792
34	1	0	1.983706	4.223404	-1.097734
35	1	0	-4.673008	-1.507688	0.410465
36	1	0	-4.497480	1.134789	-1.192885
37	1	0	-5.631112	0.795634	0.137875
38	1	0	-5.852210	0.034130	-1.436192
39	1	0	-2.561647	-0.479997	-1.586036
40	1	0	-3.618618	-1.811213	-2.075875
41	1	0	-2.524348	-2.025458	-0.706286

Rotational constants (GHZ): 0.4758382 0.2879416 0.2054336

ZPVE =952.9428 kJ mol^{-1}

E[M06-2X/6-31+G(d,p)] = -806.337147 a.u.

E[M06-2X/6-311++G(2d,p)] = -806.5500451 a.u.

Table S28. B3LYP/6-31+G(d,p) Optimized Structure for TS z_2(LK) → w_2(LK)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.230040	2.190786	-0.368905
2	6	0	-1.740184	-0.399357	1.466233
3	6	0	-2.864813	0.359407	1.397728
4	6	0	-0.559882	-0.120023	0.653422
5	8	0	-0.484664	0.871937	-0.127994
6	6	0	2.012438	-2.442993	-0.351185
7	8	0	1.544103	-3.390010	0.241988
8	8	0	2.913548	-2.540210	-1.343145
9	1	0	3.119254	-3.482086	-1.481971
10	7	0	0.476560	-0.985290	0.786678
11	1	0	0.328720	-1.834071	1.323903
12	6	0	1.677367	-0.985355	-0.035926
13	6	0	2.887112	-0.306281	0.661287
14	6	0	2.686865	1.197713	0.897716
15	6	0	2.871740	2.062175	-0.369809
16	6	0	2.072804	3.366125	-0.339792
17	7	0	0.636072	3.117843	-0.752789
18	1	0	0.022060	3.885097	-0.470756
19	1	0	0.566705	3.038627	-1.770424
20	6	0	-4.512974	-0.567250	-0.249983
21	6	0	-5.462058	0.581655	-0.356623
22	6	0	-3.676213	-0.971535	-1.417705
23	1	0	-1.700730	-1.264782	2.122744
24	1	0	-3.676110	0.206940	2.098873
25	1	0	-2.882876	1.263070	0.798935
26	1	0	1.449884	-0.474676	-0.976566
27	1	0	3.782759	-0.478571	0.054165
28	1	0	3.049184	-0.808665	1.621328
29	1	0	1.694521	1.356644	1.335410
30	1	0	3.402398	1.534799	1.655635
31	1	0	2.603419	1.504006	-1.277195
32	1	0	3.929652	2.317927	-0.489119
33	1	0	2.044835	3.794180	0.665350

34	1	0	2.476637	4.118420	-1.020980
35	1	0	-4.777729	-1.355576	0.452935
36	1	0	-5.010658	1.440063	-0.868238
37	1	0	-5.831797	0.908331	0.620977
38	1	0	-6.348623	0.295480	-0.947324
39	1	0	-3.242903	-0.104657	-1.929523
40	1	0	-4.287368	-1.510631	-2.160923
41	1	0	-2.866809	-1.647956	-1.124521

Rotational constants (GHZ): 0.4817414 0.2570742 0.1914241

ZPVE = 944.3086 kJ mol^{-1}

E[B3LYP/6-31+G(d,p)] = -806.7241589 a.u.

E[B3LYP/6-311++G(2d,p)] = -806.9186146 a.u.

E[PMP2/6-311++G(2d,p)] = -804.7371592 a.u.

E[CCSD(T)/6-31G(d)] = -804.265903 a.u.

E[MP2/6-31G(d)] = -804.04449072 a.u.

E[MP2/aug-cc-pVTZ] = -805.1415094 a.u.

E[CCSD(T)/6-311+G(2d,p)] = -804.958571 a.u.

E[CCSD(T)/aug-cc-pVTZ] = -805.362922 a.u.

Table S29. B3LYP/6-31+G(d,p) Optimized Structure for C_3H_7 radical

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.535368	-0.044815
2	6	0	-1.299403	-0.198346	0.002901
3	6	0	1.299395	-0.198360	0.002891
4	1	0	0.000025	1.612605	0.101904
5	1	0	-1.315400	-1.036853	-0.707978
6	1	0	-1.489028	-0.640124	0.998133
7	1	0	-2.148238	0.454674	-0.224055
8	1	0	1.314872	-1.037699	-0.707000
9	1	0	2.148114	0.454361	-0.225393
10	1	0	1.489696	-0.638931	0.998532

Rotational constants (GHZ): 37.2935619 8.2941955 7.4121480

ZPVE = 230.5921 kJ mol^{-1}

E[B3LYP/6-31+G(d,p)] = -118.4935378 a.u.

E[B3LYP/6-311++G(2d,p)] = -118.5181308 a.u.

E[PMP2/6-311++G(2d,p)] = -118.1272437 a.u.

E[CCSD(T)/6-31G(d)] = -118.0609994 a.u.

E[MP2/6-31G(d)] = -118.0073901 a.u.

E[MP2/aug-cc-pVTZ] = -118.1942066 a.u.

E[CCSD(T)/6-311+G(2d,p)] = -118.180853 a.u.

E[CCSD(T)/aug-cc-pVTZ] = -118.247816 a.u.

Table S30. Average Rate Constants for z_2 ion Dissociations[a]

Peptide	k_1	k_{cool}	%rmsd
AALR	1028 ± 152[b]	585 ± 88[b]	1.2
AAALR	304 ± 70	649 ± 150	1.2
AAAALR	53 ± 9	600 ± 104	1.1
AAAAALR	14	497	0.9
AAALK	250 ± 5	520 ± 20	1.2
AAAALK	87 ± 6	551 ± 50	1.2
AAAAALK	55 ± 11	650 ± 150	0.9

[a]In s^{-1}. [b]Uncertainty limits within the %rmsd fit.

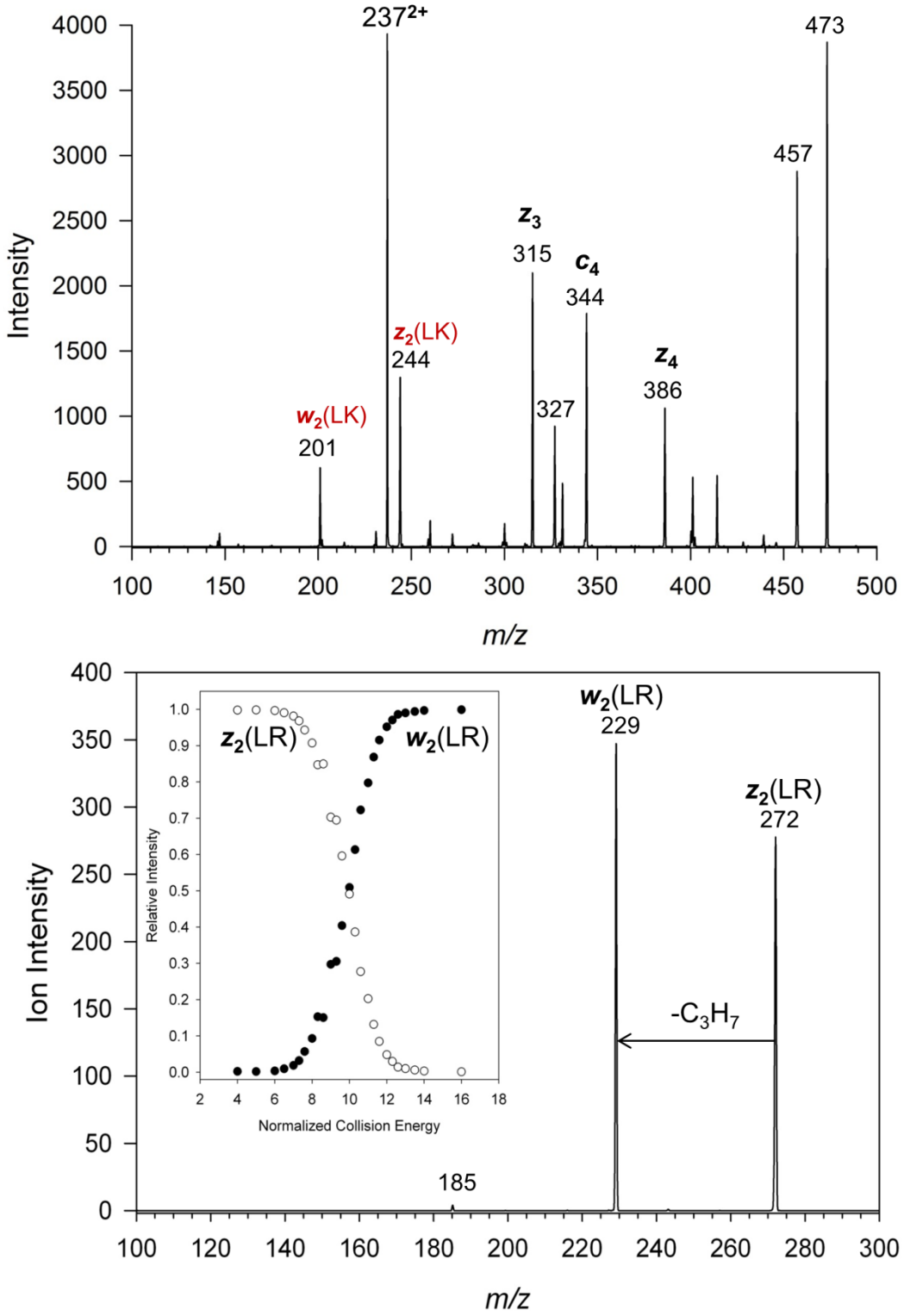

Figure S1. Representative mass spectra. Top panel: ETD mass spectrum of $(AAALK + 2H)^{2+}$, *m/z* 237, at 200 ms ion-ion interaction time. Bottom panel: CID-MS^3 mass spectrum and breakdown diagram (inset) of mass-selected $\boldsymbol{z}_2$(LR) ions (*m/z* 272) from ETD of $(AAALR + 2H)^{2+}$.

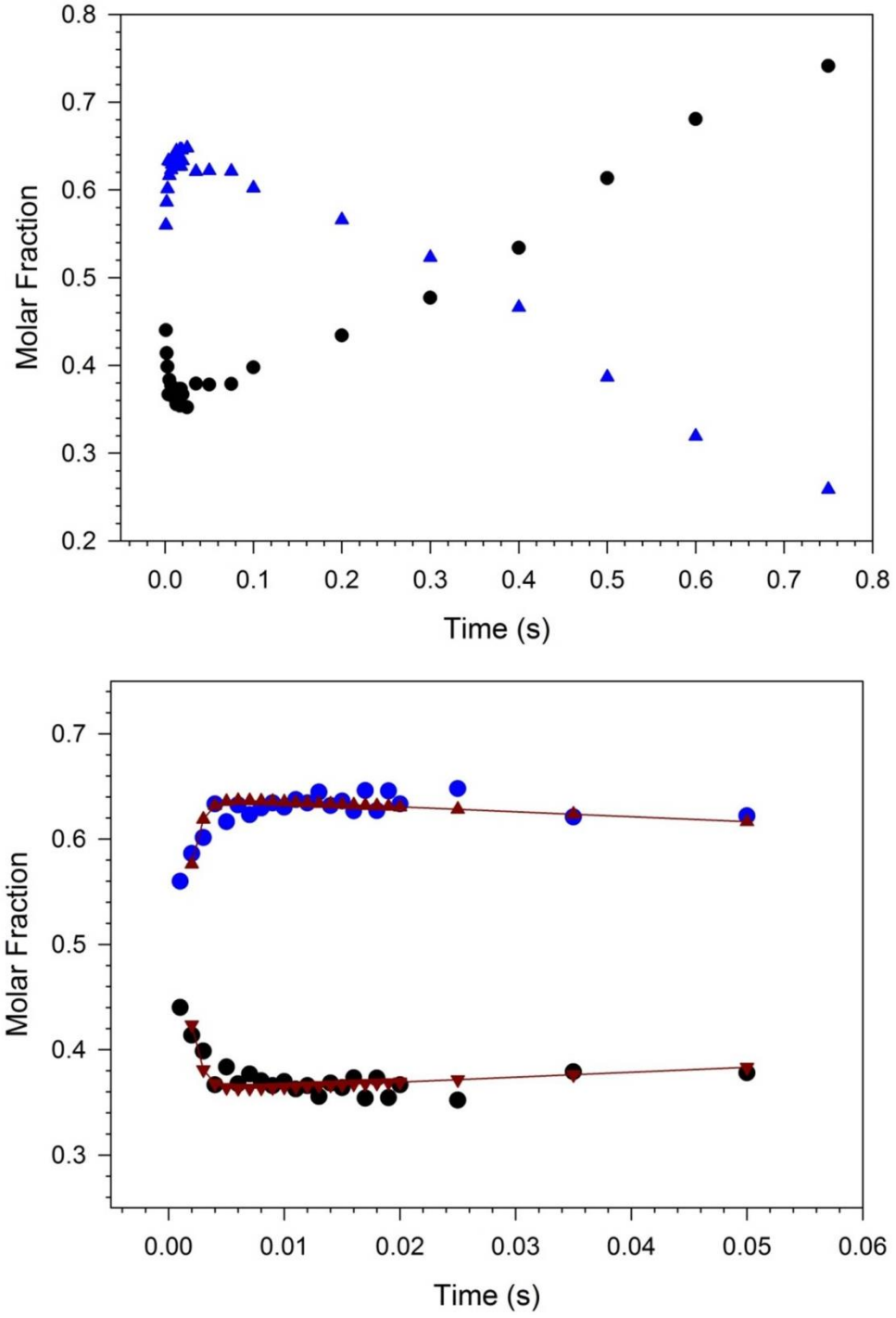

Figure S2. Top panel: Time-resolved breakdown diagram of the z_2(LR) ions from AALR. Black full circles: z_2 ions, blue triangles: w_2 ions. Bottom panel: Expanded view of the 0-50 ms interval. Black circles: z_2 ions; blue circles: w_2 ions. The red triangles and lines are the calculated molar fractions from least squares fit to eq. 6-8.

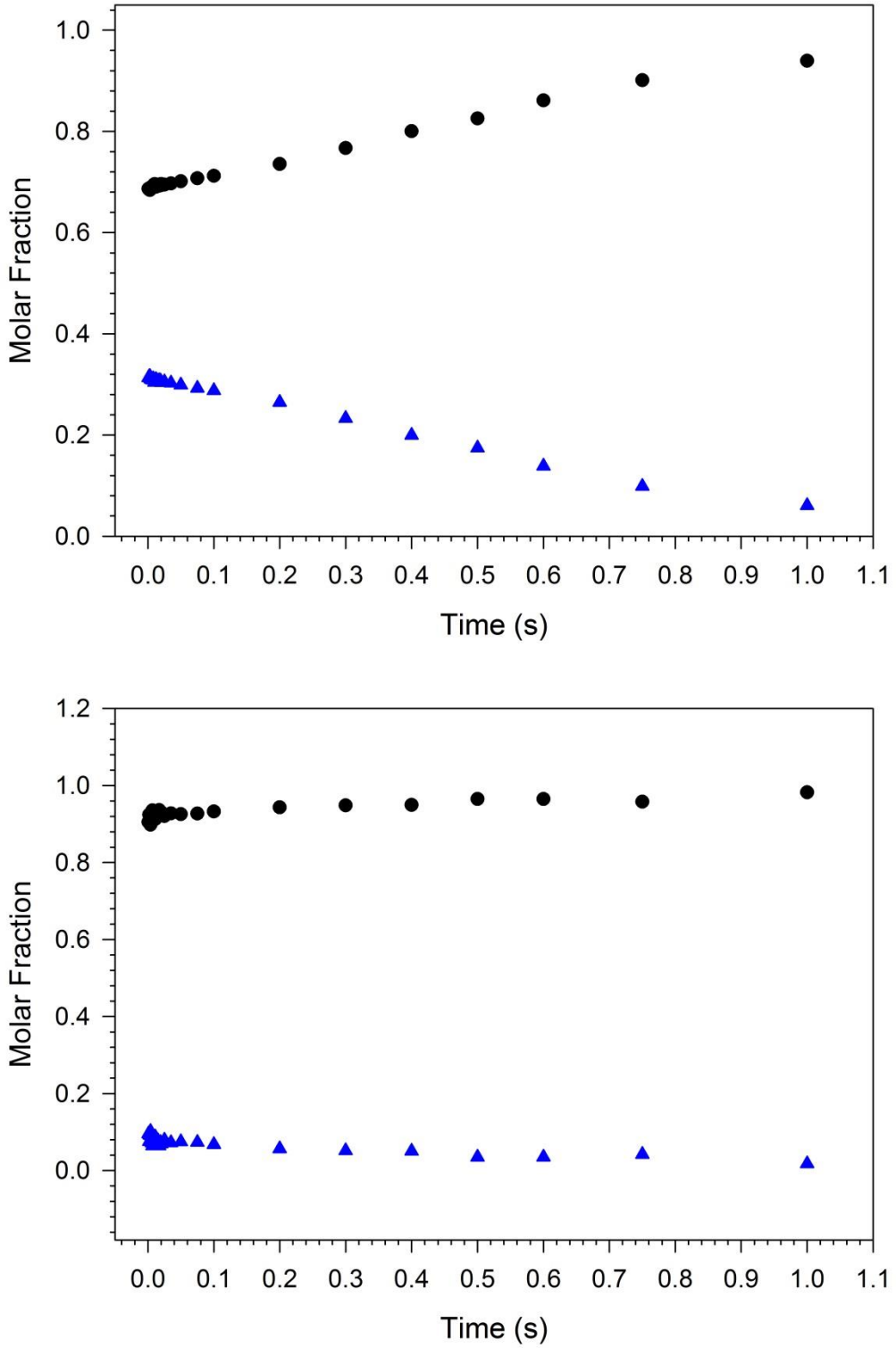

Figure S3. Time-resolved breakdown diagram of the z_2(LR) ions from (top panel) AAALR and (bottom panel) AAAALR. Black full circles: z_2 ions; blue triangles: w_2 ions.

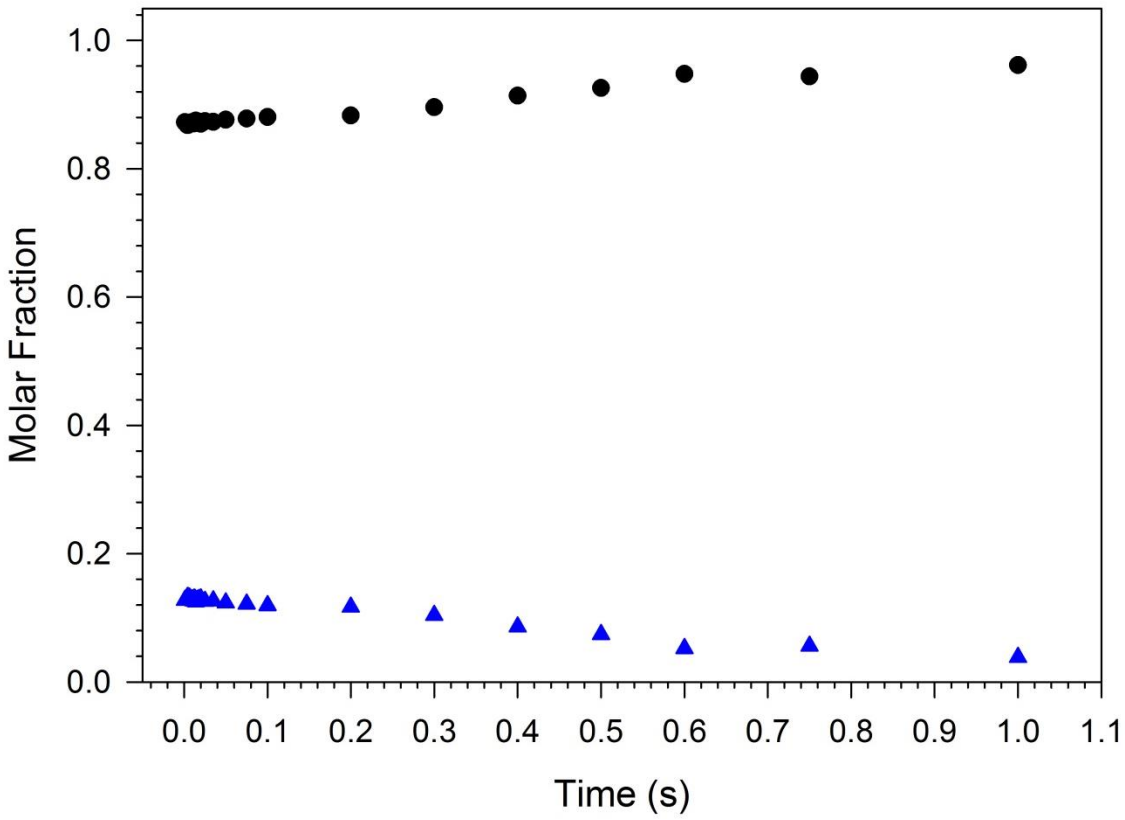

Figure S4. Time-resolved breakdown diagram of the z_2(LK) ions from AAAALK. Black full circles: z_2 ions; blue triangles: w_2 ions.

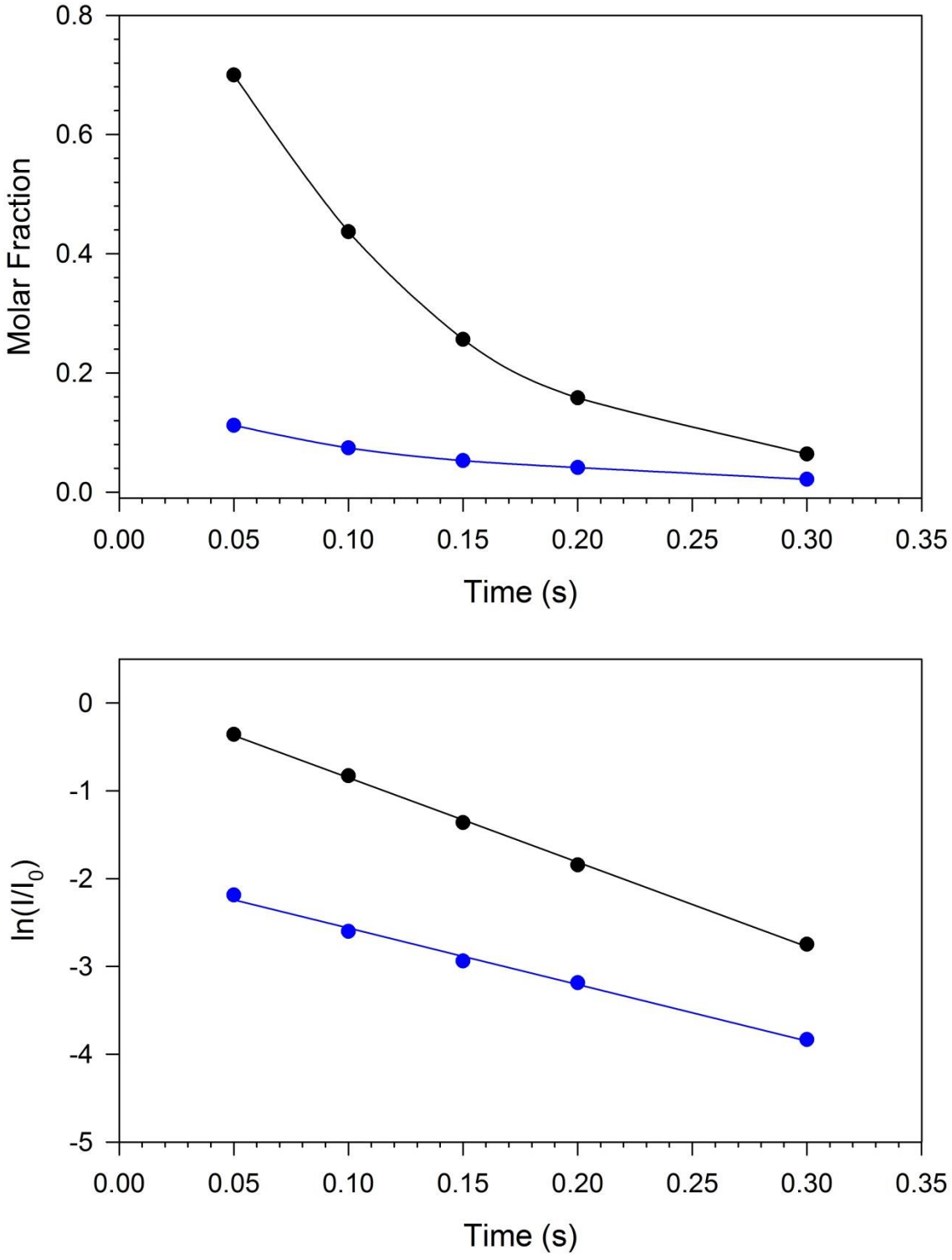

Figure S5. Depletion curves for z_2(LK) and w_2(LK) ions from AAALR. Black circles: z_2 ions; blue circles: w_2 ions.

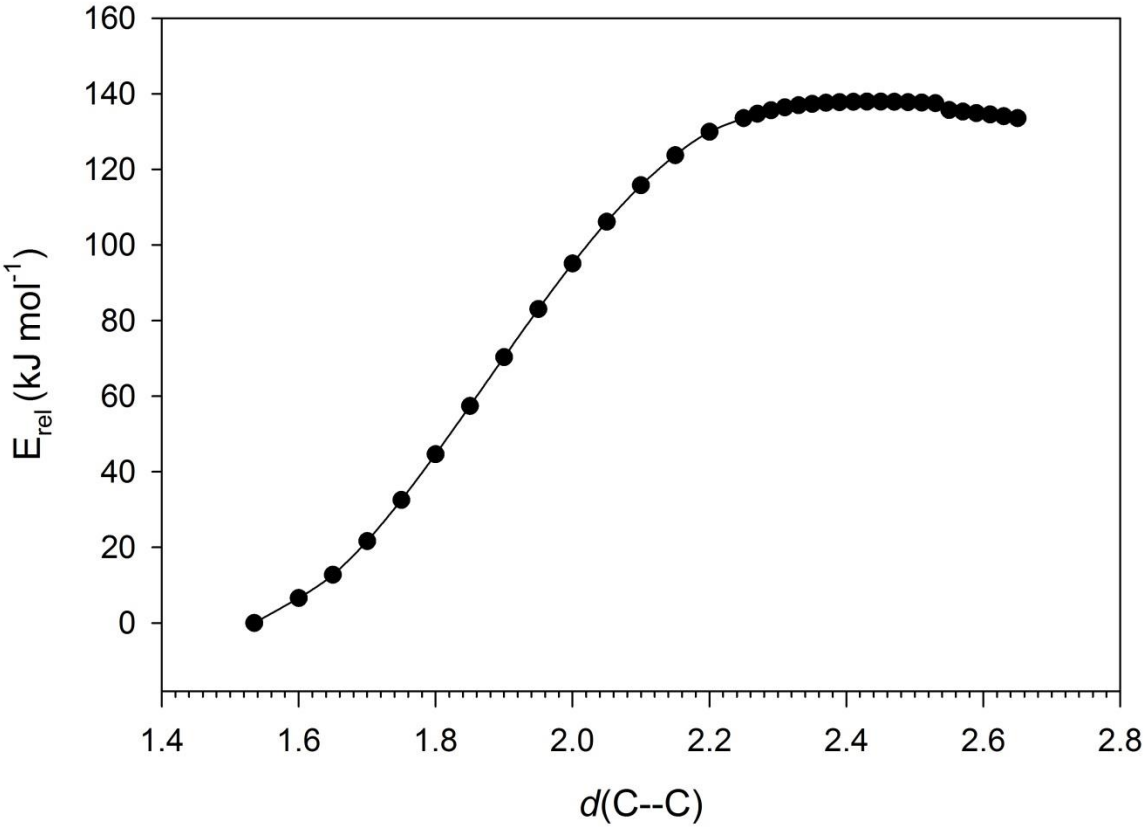

Figure S6. M06-2X/6-31+G(d,p) potential energy surface for $\mathbf{z_2}$(LR) ion dissociation by loss of C_3H_7 radical.

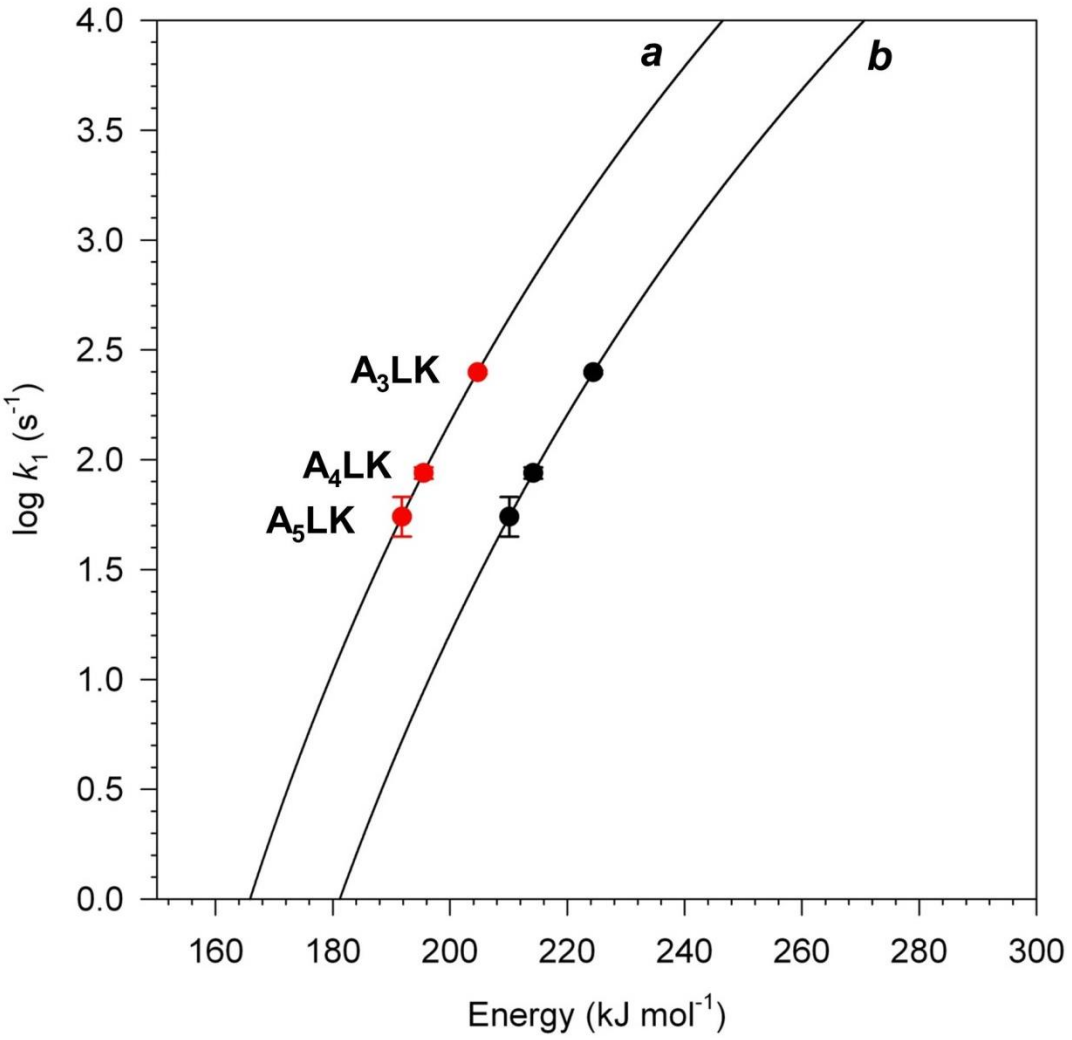

Figure S7. RRKM plots of rate constants for $\mathbf{z_2}$(LK) ion dissociations by C_3H_7 radical loss as a function of internal energy based on (a) CCSD(T)/aug-cc-pVTZ energy of the transition state, and (b) M06-2X/6-311++G(2d,p) energy for the dissociation threshold. Circles with error bars represent experimental rate constants.