Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Materials

Initial Hydration Behavior of Sodium iodide dimer: Photoelectron spectroscopy and ab initio calculations

Ren-Zhong Li,[1,2,4] Gao-Lei Hou[2], Cheng-Wen Liu,[3] Hong-Guang Xu[2], Xiang Zhao[4]*, Yi Qin Gao,[3]* Wei-Jun Zheng[2]*

[1]*College of Electronics and Information, Xi'an Polytechnic University, Xi'an 710048, China*

[2]*Beijing National Laboratory for Molecular Sciences, State Key Laboratory of Molecular Reaction Dynamics, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China*

[3]*Beijing National Laboratory for Molecular Sciences, Institute of Theoretical and Computational Chemistry, College of Chemistry and Molecular Engineering, Peking University, Beijing 100871, China*

[4]*Institute for Chemical Physics, School of Science, Xi'an Jiaotong University, Xi'an 710049, China*

**Corresponding author. Email: xzhao@mail.xjtu.edu.cn, gaoyq@pku.edu.cn, zhengwj@iccas.ac.cn,*

Tel: +86 10 62635054, Fax: +86 10 62563167

Table S1 The theoretical Na–I distances of $(NaI)_2(H_2O)_n^-$ (n=0-6) with LC-ωPBE method.

n	isomer	Na1-I1	Na1-I2	Na2-I1	Na2-I2
0	0A	2.83	2.91		3.05
	0B	2.83	2.83	3.38	3.38
1	1A	2.95	2.96		3.02
	1B	2.83	2.92		3.34
2	2A	4.59	2.94		3.04
	2B	2.97	2.97	5.12	5.12
	2C	2.98	2.92		3.05
3	3A	4.36	2.99		3.01
	3B	2.93	3.07	5.03	4.89
	3C	4.16	2.95		3.06
4	4A	3.29	3.29	4.92	4.92
	4B	3.17	3.06	4.84	4.92
5	5A	3.32	4.13	5.04	4.84
	5B	3.26	3.26	4.80	4.80
6	6A	3.42	4.32	4.98	4.99
	6B	3.28	4.15	4.93	4.72

Table S2 The theoretical Na–I distances of $(NaI)_2(H_2O)_n$ (n=0-6) with LC-ωPBE method.

n	isomer	Na1-I1	Na1-I2	Na2-I1	Na2-I2
0	0A′	2.91	2.91	2.91	2.91
1	1A′	2.94	3.05	2.89	2.90
	1B′	2.99	2.92	2.99	2.92
2	2A′	2.92	3.04	2.92	3.04
	2B′	3.02	2.93	2.93	3.02
	2C′	2.89	2.89	3.11	3.11
3	3A′	3.08	3.12	2.91	3.02
	3B′	2.96	3.30	2.90	3.04
	3C′	3.06	4.77	2.94	2.97
4	4A′	2.96	4.36	2.96	4.36
	4B′	3.07	3.07	3.07	3.07
	4C′	3.09	4.29	2.92	3.01
5	5A′	3.20	4.46	2.94	4.29
	5B′	3.06	4.32	4.34	3.01
	5C′	3.07	4.52	3.07	4.52
6	6A′	3.77	4.40	2.98	4.28
	6B′	3.17	4.41	3.17	4.41
	6C′	3.11	4.37	4.73	4.13

Table S3 The theoretical Na−I distances of $(NaI)_2(H_2O)_n^-$ (n=0-3) with MP2 method.

n	isomer	Na1-I1	Na1-I2	Na2-I1	Na2-I2
0	0A	2.84	2.92		3.03
	0B	2.84	2.84	3.25	3.25
1	1A	2.96	2.96		3.01
	1B	2.84	2.93		3.27
2	2A	2.97	2.97	5.14	5.14
	2B	4.62	2.94		3.04
	2C	2.97	2.92		3.05
3	3A	2.92	3.07	5.04	4.95
	3B	4.42	2.98		3.02
	3C	4.23	2.95		3.07

Table S4 Relative energies of the low energy isomers of $(NaI)_2(H_2O)_n^-$(n = 0-3) as well as the comparison of their theoretical VDEs to the experiments. The 6-311++G** basis set was used for Na, O and H atoms. The LANL2DZdp ECP basis set was used for iodine atom.

isomer		ΔE* (eV)	Sym.	State	Theo.(MP2)	Expt.
					VDE (eV)	VDE (eV)
$(NaI)_2^-$	0A	0.00	C_s	^2A	1.61	1.70
	0B	0.25	C_{2v}	$^2A_1$	0.47	
$(NaI)_2(H_2O)^-$	1A	0.00	C_1	^2A	1.55	1.62
	1B	0.17	C_1	^2A	1.32	1.24
$(NaI)_2(H_2O)_2^-$	2A	0.00	C_2	^2A	1.38	1.18
	2B	0.03	C_1	^2A	1.66	1.62
	2C	0.03	C_1	^2A	1.66	
$(NaI)_2(H_2O)_3^-$	3A	0.00	C_1	^2A	1.01	1.04
	3B	0.01	C_1	^2A	1.51	1.59
	3C	0.03	C_1	^2A	1.06	

* The ΔE values are from the MP2 method.

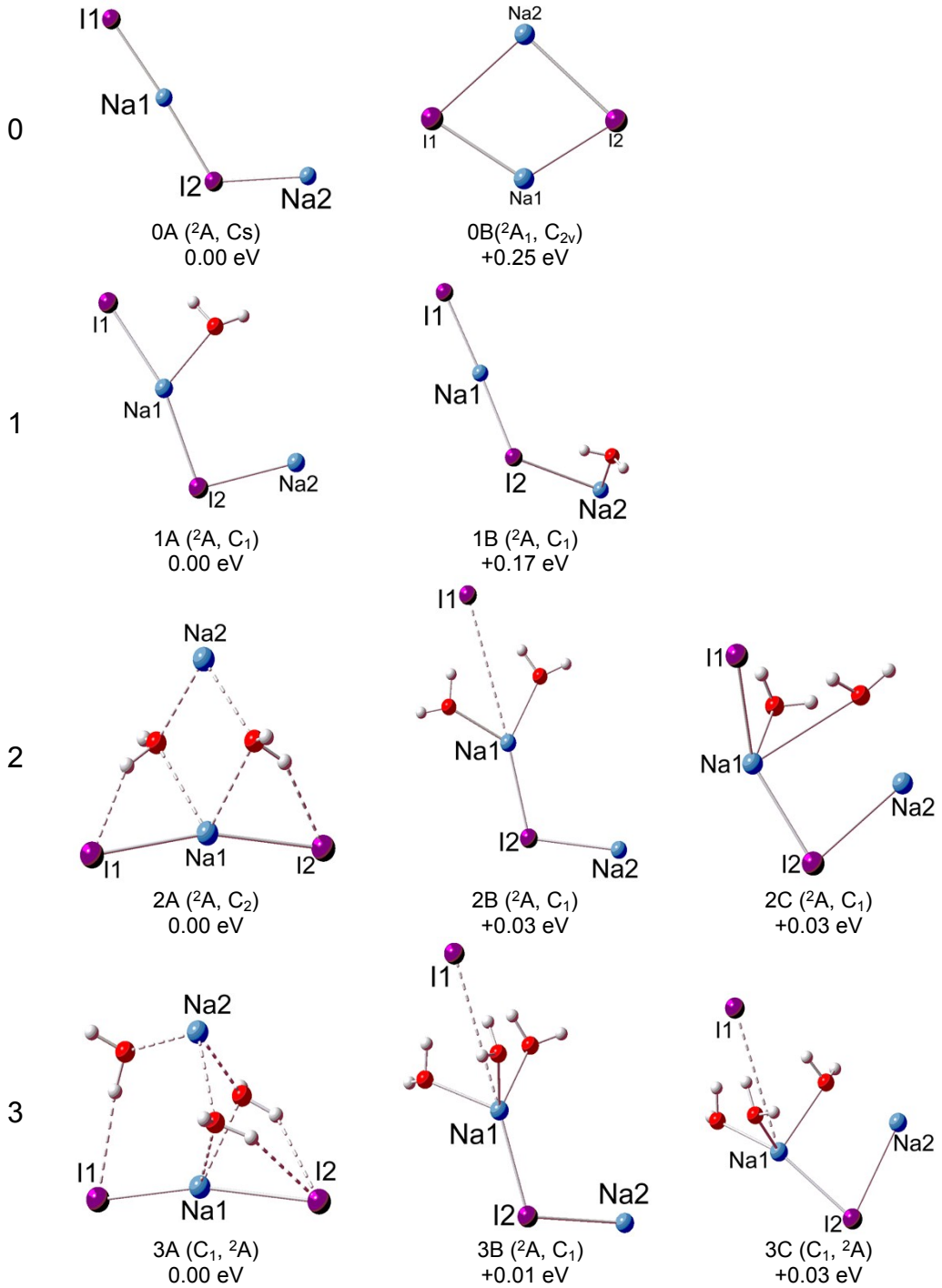


Figure S1. Optimized geometries of the low-lying isomers of $(NaI)_2(H_2O)_n^-$ (n = 0-3) clusters with MP2 method.

Table S5. The Cartesian atomic coordinates of the typical low-lying isomers of $(NaI)_2(H_2O)_n^{0/-}$ (n=0-6) clusters optimized with LC-ωPBE functional.

$(NaI)_2^-$

0A

I	3.265810	0.140570	-0.000009
I	-2.440185	-0.498283	-0.000008
Na	0.442441	-0.092865	0.000085
Na	-4.420451	1.816389	-0.000003

0B

I	0.000000	2.474356	0.661440
I	0.000000	-2.474356	0.661440
Na	0.000000	0.000000	2.032983
Na	0.000000	0.000000	-1.640112

$(NaI)_2(H_2O)^-$

1A

I	3.141080	-0.194652	0.231648
I	-2.684436	-0.668094	-0.093863
O	0.704713	2.198033	-0.320967
H	1.646565	2.052956	-0.132872
H	0.451003	3.047610	0.045160
Na	0.210703	-0.062109	-0.114994
Na	-3.355124	2.249669	0.280439

1B

I	-3.595280	-1.365239	0.995687
I	1.443076	-0.070061	-1.434145
Na	-1.142366	-0.624090	-0.204988
Na	3.477064	2.559461	-1.075009
O	3.884604	1.051216	0.722286
H	3.254855	0.365909	0.446766
H	4.719823	0.611580	0.894682

$(NaI)_2(H_2O)_2^-$

2A

I	-3.970352	0.621677	0.411948
I	3.513598	-0.085177	0.839259
O	-1.111823	-0.938879	1.483559
H	-1.994281	-0.578538	1.238220
H	-1.280662	-1.709070	2.026865
O	-0.805317	1.704638	-0.379817
H	-1.753722	1.495224	-0.223581
H	-0.791673	2.487829	-0.930943
Na	5.066371	2.041308	-0.671532
Na	0.602930	0.255472	0.626895

2B

I	-2.697802	0.137913	0.613044
I	2.964441	-1.233268	-0.055198
O	-0.417530	1.892126	-1.172424
H	-1.281890	1.658380	-0.765964
H	-0.562450	1.882372	-2.122502
Na	0.233092	-0.109178	0.224618
Na	1.058000	3.516063	-0.224810
O	1.747906	1.687391	1.150843
H	2.407217	1.020029	0.856048
H	1.924898	1.837814	2.083470

2C

I	2.563955	0.008519	-2.112535
I	-2.930999	-0.422095	-1.173177
O	0.608824	1.135487	0.636635
H	1.231454	1.149012	-0.116272
H	0.883532	1.843304	1.234472
Na	-0.100690	-1.114853	-1.373320
Na	-1.777259	1.667820	0.730708
O	1.079100	-1.755985	0.589928
H	1.937993	-1.584050	0.179372
H	0.897262	-0.945827	1.086079

$(NaI)_2(H_2O)_3^-$

3A

I	4.310497	-0.388311	-0.181583
I	-3.034043	-0.490745	0.062235
O	1.294454	1.074875	-1.247122
H	2.215529	0.857864	-1.007931
H	1.302315	1.213362	-2.195595
O	1.409483	-0.152574	1.798936
H	2.314307	-0.236853	1.443412
H	1.453318	0.529607	2.470930
O	1.326930	-2.158696	-0.774797
H	1.382593	-3.036338	-0.392907
H	2.236218	-1.805120	-0.744385
Na	-4.137707	0.757898	2.572803
Na	-0.048557	-0.406605	-0.013287

3B

I	-3.211278	-0.594914	-0.720106
I	2.425114	-1.014930	0.661350
O	-0.864149	1.793344	-1.542087
H	-1.775274	1.446845	-1.593127
H	-0.722844	2.340435	-2.321659
Na	-0.180589	-0.238335	-0.421248
Na	-0.326428	3.192735	0.398806
O	1.750289	2.404059	1.061102
H	2.025874	1.466649	1.036405
H	2.546835	2.916656	0.905357
O	-1.157037	1.167858	1.400668
H	-0.935113	0.851064	2.280288
H	-2.014677	0.772909	1.154193

3C

I	3.449212	0.165549	-0.160528
I	-3.363816	-0.235163	-0.121939
O	0.239407	1.396564	0.696225
H	1.125695	1.287489	0.296275
H	0.400419	1.918527	1.491266
O	1.209144	-1.763081	1.693235
H	1.982865	-1.362912	1.246656
H	1.405237	-1.715358	2.630193
O	0.591284	-1.201994	-1.581381
H	0.284636	-0.804211	-2.398457
H	1.510374	-0.901568	-1.453599
Na	-1.973387	2.474313	0.201761
Na	-0.536254	-0.891953	0.420051

$(NaI)_2(H_2O)_4^-$

4A

I	2.845270	-0.711695	0.159425
I	-2.397062	-0.888297	-1.583375
O	1.153952	1.977730	1.418538
H	1.938645	1.433227	1.202509
H	1.370786	2.505828	2.192294
Na	-0.277389	0.160648	0.699144
Na	-0.063261	3.232256	-0.255961
O	-1.961557	1.872806	0.382735
H	-2.426483	1.286234	-0.248669
H	-2.629580	2.371013	0.862460
O	0.414500	1.268885	-1.494267
H	-0.232133	0.715946	-1.962636
H	1.244866	0.765673	-1.471581
O	-0.355830	-2.138216	1.167990
H	-0.912918	-2.369754	0.412160
H	0.555436	-2.320400	0.900344

4B

I	3.378418	-0.379180	-0.755414
I	-1.993518	-0.969632	-2.268931
O	1.160850	0.882622	1.508873
H	2.032617	0.727325	1.090075
H	1.288212	0.797469	2.457369
Na	0.402039	-0.793166	-0.203030
Na	-0.330684	2.533630	0.633968
O	-2.242519	1.068125	0.541554
H	-2.426223	0.669627	-0.333386
H	-3.002258	1.612731	0.776113
O	0.417276	1.488551	-1.365144
H	-0.153267	1.127844	-2.060192
H	1.334903	1.293966	-1.612787
O	-1.333374	-1.583705	1.215500
H	-1.734595	-0.718254	1.387035
H	-1.885571	-1.951243	0.513607

$(NaI)_2(H_2O)_5^-$

5A

I	3.001839	-0.739127	-0.210776
I	-3.125030	-0.408754	0.096437
O	1.607052	2.226010	0.870455
H	2.194524	1.491155	0.583423
H	2.166121	2.868588	1.315826
Na	-0.395444	1.025117	1.335295
Na	0.251911	3.175006	-0.959225
O	-1.736176	2.775607	0.361823
H	-2.432495	2.132892	0.127592
H	-2.170988	3.594566	0.618100
O	0.006652	0.822473	-1.153890
H	-0.781932	0.284666	-1.314446
H	0.782702	0.233821	-1.193850
O	0.093638	-1.322266	1.663755
H	-0.554747	-1.700608	1.057019
H	0.969032	-1.451635	1.255326
O	-1.567883	0.309246	3.327069
H	-1.043484	-0.498951	3.252885
H	-2.375161	0.107909	2.833588

5B

I	2.732552	-0.941782	-0.120939
I	-2.762741	-0.711958	-0.211705
O	1.730258	2.216052	0.689913
H	2.374008	1.512883	0.466447
H	2.174271	2.848202	1.263934
Na	0.020517	0.480525	0.989126
Na	0.158476	3.042900	-0.880480
O	-1.527666	2.352258	0.636186
H	-2.220135	1.704937	0.390693
H	-1.936024	3.020010	1.196195
O	0.078292	0.840065	-1.599140
H	-0.724077	0.292624	-1.638732
H	0.833077	0.227557	-1.612971
O	-0.083920	-1.569212	2.121272
H	-0.865063	-1.905098	1.661577
H	0.681188	-1.969734	1.687087
O	0.259439	5.287066	-1.315564
H	1.036131	5.751763	-0.965019
H	-0.486840	5.815454	-0.990068

$(NaI)_2(H_2O)_6^-$

6A

I	3.124471	-0.937542	-0.363810
I	-3.114406	-0.576549	-0.653723
O	2.444338	2.545155	-0.119876
H	2.819880	1.676048	-0.361037
H	3.102941	3.211433	-0.338650
Na	-0.562300	0.499826	1.357626
Na	0.233491	3.095083	-0.902555
O	-1.710828	2.448150	0.453703
H	-2.357754	1.862655	0.014229
H	-2.200362	3.207006	0.785428
O	0.126025	0.750450	-1.076965
H	-0.634685	0.245432	-1.403775
H	0.915072	0.184336	-1.153424
O	-0.095253	-1.862694	1.021208
H	-0.697265	-2.041020	0.287356
H	0.806031	-1.938411	0.668354
O	-2.097865	-0.685383	2.796379
H	-1.556464	-1.475762	2.685240
H	-2.772860	-0.764232	2.106207
O	1.541015	1.090726	2.182308
H	2.120542	0.379267	1.869619
H	1.878926	1.864865	1.709912

6B

I	3.152417	-1.007448	-0.324549
I	-2.973284	-0.761590	-0.650136
O	1.531542	1.491020	1.379582
H	2.173976	0.857411	0.985004
H	1.978269	1.918285	2.116046
Na	-0.487049	0.193584	1.257364
Na	0.389877	2.819362	-0.269039
O	-1.703757	2.217691	0.665872
H	-2.377252	1.685581	0.202551
H	-2.163652	2.901369	1.165469
O	0.224170	0.692909	-1.171844
H	-0.543269	0.212117	-1.516782
H	1.008062	0.120023	-1.263337
O	0.077853	-2.130505	0.947874
H	-0.479064	-2.338042	0.187784
H	0.999138	-2.139031	0.631098
O	-1.824617	-1.065746	2.815657
H	-1.277188	-1.825415	2.578598
H	-2.577789	-1.121051	2.211939
O	0.775516	5.065105	-0.447945
H	0.030784	5.592151	-0.110336
H	1.547558	5.455363	-0.012126

$(NaI)_2$

0A′

I	1.218115	1.547531	0.000095
I	-2.794313	-0.864635	0.000074
Na	0.100775	-1.137088	-0.000247
Na	-1.676962	1.820003	0.000143

$(NaI)_2(H_2O)$

1A′

I	-2.491972	0.030402	-0.012904
I	2.196198	-0.557426	0.049069
Na	-0.363262	-1.923819	-0.018556
Na	0.009626	1.564375	0.057166
O	1.790190	2.983776	0.113578
H	2.522764	2.353365	0.112476
H	2.163716	3.866338	0.137110

1B′

I	-2.559265	-0.517314	-0.228488
I	2.240380	0.457337	-0.578951
O	-0.737031	1.755171	1.348399
H	-1.685970	1.582298	1.435499
H	-0.498239	2.477320	1.936437
Na	0.112872	-0.609077	1.119695
Na	-0.463787	1.419149	-1.136895

$(NaI)_2(H_2O)_2$

2A′

I	1.564849	1.531923	0.713040
I	-2.837514	-0.128869	-0.008195
O	0.489353	3.161240	-2.242207
H	1.278162	3.144383	-1.683599
H	0.653824	3.771031	-2.963271
Na	-0.568803	-0.335163	1.813929
Na	-0.847765	1.683920	-1.132665
O	1.023850	-0.707311	3.403394
H	1.730078	-0.126456	3.089714
H	1.332187	-1.138779	4.201889

2B′

I	2.154633	0.092986	0.022815
I	-2.603135	0.248738	0.027427
O	-1.846690	-3.218644	0.065744
H	-2.631480	-2.653737	0.060428
H	-2.141575	-4.130613	0.076510
Na	-0.223051	1.958410	0.004841
Na	-0.225455	-1.616685	0.045307
O	1.398195	3.560340	-0.016777
H	2.182976	2.995419	-0.011489
H	1.693098	4.472296	-0.028145

2C′

I	-2.384699	-0.424935	-0.192219
I	2.384696	-0.424937	0.192208
O	1.462763	2.521052	-1.493962
H	1.599271	3.078125	-2.261821
H	2.186943	1.881051	-1.460434
Na	0.000009	-2.036881	0.000038
Na	-0.000023	1.563068	-0.000011
O	-1.462734	2.521043	1.493996
H	-1.599212	3.078133	2.261848
H	-2.186966	1.881102	1.460458

$(NaI)_2(H_2O)_3$

3A′

I	-1.958122	0.376067	1.010481
I	2.043703	-0.199098	-1.591373
O	-1.943583	-3.032889	0.097256
H	-2.503412	-2.416132	0.589058
H	-2.348469	-3.900282	0.145258
O	-1.246185	3.411493	-0.593887
H	-2.001819	2.886886	-0.295159
H	-1.574989	4.079832	-1.197073
O	2.601672	2.372018	0.726111
H	3.149592	2.652472	1.460733
H	3.065199	1.656143	0.268897
Na	0.477052	1.974968	-0.071164
Na	-0.278094	-1.602594	-0.527762

3B′

I	-2.224092	0.043394	0.134880
I	2.612250	0.210702	-0.231990
O	-1.386863	3.468136	-0.088879
H	-2.184926	2.928927	-0.004198
H	-1.654600	4.388217	-0.112403
O	-0.771888	-2.569149	-1.771311
H	-1.541818	-1.988385	-1.693595
H	-0.647176	-2.751516	-2.704363
O	-0.488727	-2.389174	2.042472
H	-0.226553	-2.484109	2.959887
H	-1.265724	-1.812903	2.025005
Na	0.485705	-1.832217	0.022184
Na	0.216093	1.841592	-0.131096

3C′

I	3.438681	-0.321193	-0.059872
I	-2.364529	-0.387132	0.495982
O	1.001365	1.520055	1.424488
H	1.915680	1.277192	1.169535
H	0.989641	1.581624	2.383214
Na	0.536231	-0.846080	0.302619
Na	-0.675644	2.092515	-0.088277
O	-2.737986	3.072225	-0.062950
H	-3.246540	2.268730	0.122738
H	-3.356248	3.801492	-0.130272
O	0.717257	1.000110	-1.603243
H	0.530527	0.741493	-2.509517
H	1.669692	0.827000	-1.452055

$(NaI)_2(H_2O)_4$

4A′

I	-3.384896	0.077838	-0.000019
I	3.173429	-0.260144	-0.000024
O	-1.086549	2.809491	-0.000055
H	-1.884877	2.251625	-0.000020
H	-1.387797	3.719572	-0.000222
O	-0.331268	-0.079634	-1.530534
H	-1.300776	-0.029658	-1.402431
H	-0.167045	-0.088176	-2.476974
O	-1.379516	-2.875629	0.000049
H	-1.772712	-3.749926	0.000059
H	-2.116275	-2.238662	0.000036
O	-0.331316	-0.079451	1.530602
H	-1.300815	-0.029492	1.402417
H	-0.167169	-0.087802	2.477057
Na	0.757109	1.443922	-0.000067
Na	0.594746	-1.706810	0.000173

4B′

I	1.681666	-0.030006	0.009448
I	-3.143714	-0.074999	0.034586
O	0.646247	-2.985970	1.574890
H	1.378880	-2.354683	1.587533
H	0.698014	-3.508499	2.376603
O	-2.092045	2.872348	1.605449
H	-2.824546	2.241005	1.622228
H	-2.135547	3.390575	2.410439
O	0.575125	2.905914	-1.545014
H	0.608919	3.429410	-2.347055
H	1.319242	2.288412	-1.565339
O	-2.053513	-3.002050	-1.547948
H	-2.797809	-2.384498	-1.557055
H	-2.095726	-3.521127	-2.352459
Na	-0.713315	-1.956436	0.016484
Na	-0.748746	1.851434	0.027386

4C′

I	2.327454	1.060789	-0.495701
I	-2.662646	-0.385672	0.054788
O	3.642909	-2.196735	-0.232322
H	3.932708	-1.282746	-0.357464
H	4.422859	-2.753363	-0.230526
Na	-0.517290	1.689547	-0.344864
Na	1.366633	-1.843688	-0.094926
O	-0.277002	-2.381966	-1.615222
H	-1.111553	-1.966814	-1.336722
H	-0.308571	-2.435676	-2.572008
O	-0.016104	-2.005391	1.739303
H	-0.890370	-1.647536	1.506950
H	0.099678	-1.846533	2.677748
O	-2.319413	3.098705	-0.362440
H	-3.037802	2.464381	-0.235401
H	-2.705655	3.973244	-0.430334

$(NaI)_2(H_2O)_5$

5A′

I	3.215986	-0.341298	0.378705
I	-3.418625	-0.113008	-0.141695
O	2.500741	3.036140	0.184045
H	3.185331	2.353321	0.264974
H	2.936144	3.889437	0.182205
Na	0.578351	-1.633691	0.228921
Na	0.691401	1.604739	0.103885
O	-0.456149	0.044744	1.600514
H	-1.412904	0.046594	1.393500
H	-0.372936	0.091653	2.556278
O	-0.223721	-0.079898	-1.417582
H	-1.200844	-0.067104	-1.360083
H	0.004879	-0.110970	-2.349990
O	-1.301653	-2.935149	0.137818
H	-2.071255	-2.343336	0.054085
H	-1.641687	-3.831231	0.148768
O	-1.316242	2.749865	-0.098044
H	-1.664386	3.640571	-0.161669
H	-2.080098	2.148587	-0.132019

5B′

I	-3.387015	-0.207185	-0.097345
I	3.218456	-0.167153	-0.365864
O	-0.462630	0.565341	1.717914
H	-1.357689	0.917955	1.801575
H	0.144549	1.101626	2.246796
Na	0.603015	1.427889	-0.316436
Na	-0.778350	-1.497522	0.675344
O	1.149404	-2.668975	0.931932
H	1.876143	-2.094145	0.620745
H	1.557611	-3.463032	1.280096
O	-0.160390	-0.560013	-1.441058
H	0.546736	-0.899822	-2.000461
H	-0.990769	-0.551310	-1.934085
O	-1.342056	2.513123	-0.848395
H	-1.742719	3.299971	-1.221158
H	-2.066194	1.869658	-0.709681
O	1.827953	2.146866	1.756356
H	2.266086	2.916425	2.126493
H	2.530314	1.537809	1.457764

5C′

I	-3.329667	0.099744	-1.274049
I	2.624281	-0.225763	1.505256
O	-1.378610	2.431168	0.386138
H	-2.067859	1.879440	-0.037993
H	-1.838109	3.013551	0.993302
O	2.740960	2.597822	-0.559341
H	3.264764	3.371247	-0.774215
H	3.306652	1.985562	-0.066434
O	0.014900	-0.094292	-1.483314
H	-0.970337	-0.038102	-1.571458
H	0.357384	-0.119726	-2.381221
O	-1.658117	-2.419070	0.417081
H	-2.181018	-2.937045	1.031275
H	-2.279736	-1.797228	-0.014498
O	2.414334	-3.069713	-0.523718
H	2.845700	-3.900753	-0.728713
H	3.047017	-2.520367	-0.038172
Na	0.712403	1.655797	0.004130
Na	0.507821	-1.893999	0.026618

$(NaI)_2(H_2O)_6$

6A′

I	3.512601	-0.219117	0.288881
I	-3.347875	-0.430382	-0.107844
O	-1.830515	1.915797	1.948960
H	-2.328893	2.566362	2.447671
H	-2.482818	1.280437	1.595403
O	-1.850354	2.262958	-1.716307
H	-2.334811	2.957647	-2.165469
H	-2.491256	1.553027	-1.527603
O	0.288651	0.045885	1.567941
H	1.257094	-0.000539	1.650288
H	-0.079091	0.432212	2.369494
O	1.232240	-2.901955	0.063817
H	1.516171	-3.814834	0.130545
H	2.033722	-2.351991	0.135251
O	0.516527	0.103606	-1.405728
H	1.474368	0.025745	-1.222838
H	0.413496	0.277324	-2.344805
O	1.732928	2.820868	0.277568
H	2.398930	2.109152	0.302311
H	2.218946	3.646837	0.282633
Na	-0.353888	1.863936	0.036901
Na	-0.567831	-1.495248	0.005048

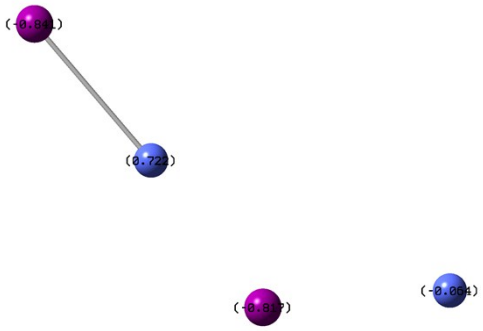
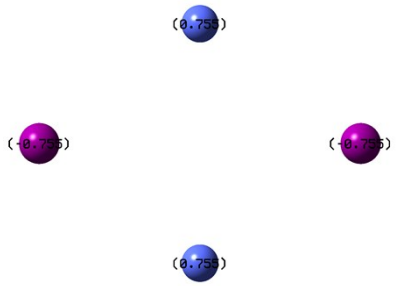
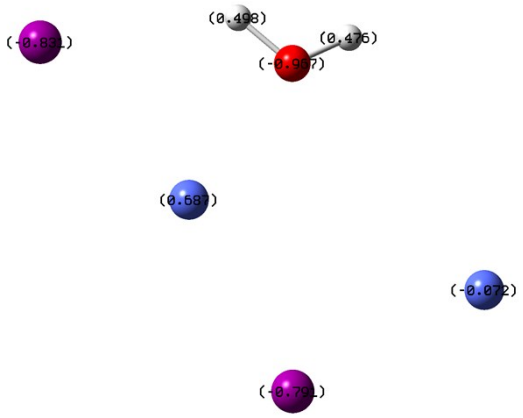
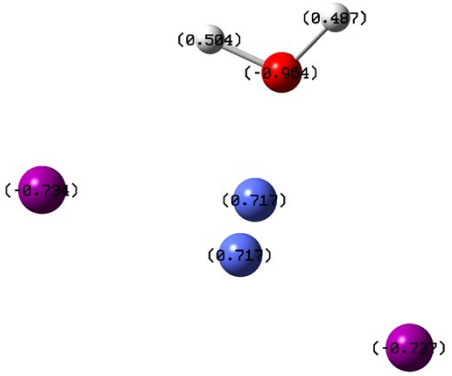
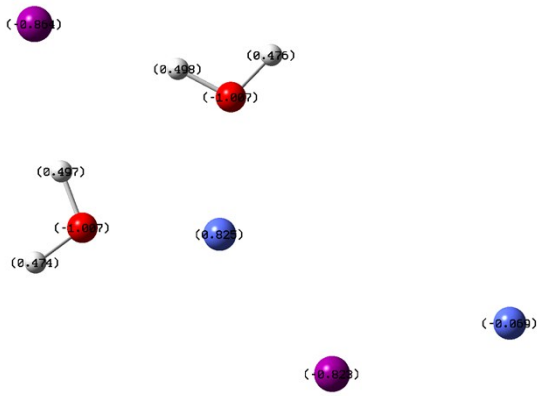
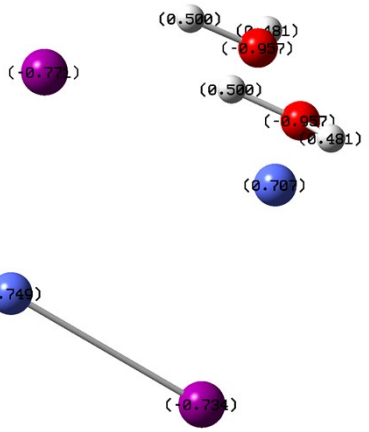
6B′

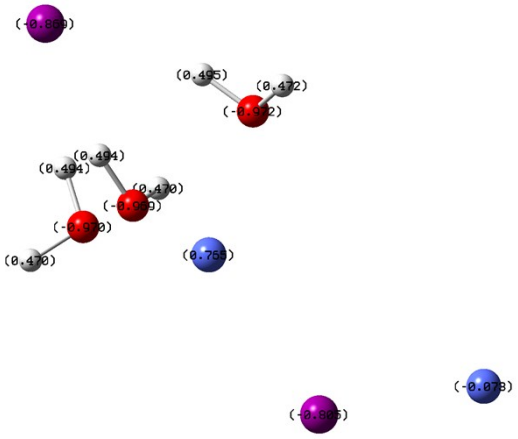
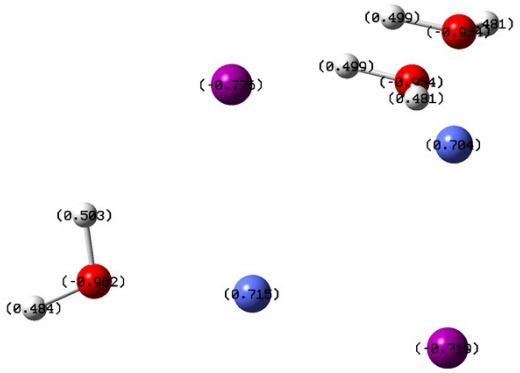
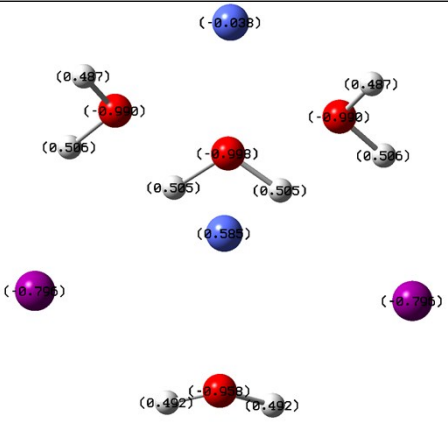
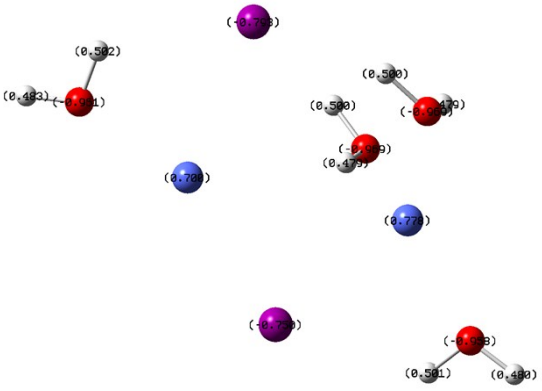
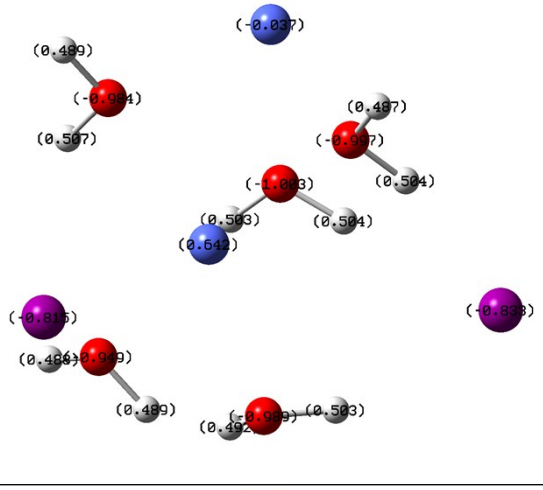
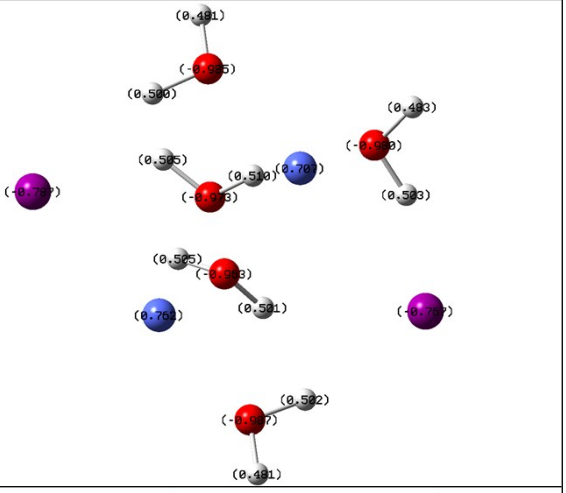
I	3.532894	0.001629	-0.050663
I	-3.202092	0.000322	-0.379600
O	0.451697	0.001990	1.541580
H	1.409094	0.002013	1.333633
H	0.378167	0.002594	2.499106
Na	-0.547872	-1.662616	0.089205
Na	-0.548448	1.664596	0.087324
O	-2.199324	2.957886	1.098863
H	-2.934884	2.355280	0.906182
H	-2.573888	3.822033	1.275556
O	0.373446	0.000247	-1.436457
H	0.122085	-0.000329	-2.363700
H	1.349271	0.000442	-1.395435
O	1.433778	-2.837323	-0.128788
H	1.796354	-3.717212	-0.015609
H	2.190785	-2.225315	-0.146145
O	-2.198520	-2.955799	1.101250
H	-2.572804	-3.820041	1.278076
H	-2.934248	-2.353593	0.907960
O	1.432760	2.839752	-0.132128
H	1.795049	3.719949	-0.020433
H	2.189978	2.227985	-0.148715

6C′

I	3.368738	-0.416611	-0.459387
I	-3.359819	-0.177354	-0.722832
O	2.573152	2.997626	-0.586846
H	3.038988	2.142421	-0.646888
H	3.132913	3.648357	-1.013378
Na	-0.759419	-0.491680	0.962569
Na	0.465999	2.475104	0.095030
O	-1.698725	2.509210	0.848563
H	-2.324274	2.078664	0.238622
H	-1.954472	2.159613	1.711578
O	0.058066	0.536271	-1.119612
H	-0.717361	0.277485	-1.638472
H	0.845650	0.083522	-1.459249
O	0.656741	-2.306668	0.837805
H	0.552727	-3.228125	0.592818
H	1.524131	-2.027128	0.496723
O	-2.474847	0.234053	2.528352
H	-2.855867	-0.046793	3.363541
H	-3.136783	0.051339	1.832483
O	1.112190	0.860700	1.752014
H	1.880071	0.460469	1.282670
H	1.384890	0.958363	2.667650

Figure S2 Natural Population Analysis (NPA) Charge Distributions of the most stable isomers of $(NaI)_2(H_2O)_n^-$(n=0-6) and their corresponding neutrals.

n	anion	neutral
0		
1		
2		

n	anion	neutral
3		
4		
5		
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