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The Simultaneous Recognition Mechanism of Cations and Anions from Macrocyclic-Iodine Structures: Insights from Dispersion corrected-DFT Calculations

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Supplementary Material

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Table S1. Optimized Cartesian coordinates of the compounds investigated from the ω B97XD/def2-TZVP computational model.

Complex		Na-1-I		
Atom	X	Y	Z	
Na	1.952561	0.577516	0.408865	
C	2.324649	3.758123	0.646062	
O	1.225737	2.876222	0.592513	
O	3.576587	2.138464	-0.560082	
C	3.176927	3.495241	-0.566608	
O	3.158929	-0.416495	-1.680859	
C	4.406274	0.251221	-1.757211	
C	4.181485	1.737707	-1.771597	
N	1.571899	-2.476443	-0.410020	
C	1.928943	-2.459349	-1.820114	
C	3.255997	-1.775921	-2.052107	
C	0.223270	3.109654	1.560019	
C	-0.727909	1.939509	1.501825	
O	-0.090676	0.741738	1.914169	
C	-0.334175	0.414695	3.272050	
N	2.458631	-2.907348	0.481802	
N	1.922287	-2.807374	1.656924	
C	0.667229	-2.310172	1.543902	
C	0.424020	-2.094857	0.205526	
C	0.303173	-0.909722	3.621826	
C	-0.174687	-2.084380	2.752977	
I	-1.266524	-1.361358	-0.751057	
I	-4.123244	0.112972	-2.330581	
H	2.895119	3.594886	1.568720	
H	1.989890	4.800982	0.627904	
H	2.596174	3.703233	-1.472487	
H	4.051809	4.154513	-0.556382	
H	4.926545	-0.023212	-2.681071	
H	5.037474	-0.040506	-0.909529	
H	5.144482	2.244229	-1.904519	
H	3.533350	2.002351	-2.615031	
H	1.979669	-3.484280	-2.187000	
H	1.135177	-1.942561	-2.355665	
H	4.041731	-2.272455	-1.474981	
H	3.503691	-1.858326	-3.115822	
H	0.670336	3.193463	2.558368	
H	-0.308332	4.042211	1.339945	
H	-1.608930	2.139852	2.116866	

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H	–1.061258	1.790782	0.472475
H	0.054978	1.203611	3.926923
H	–1.418139	0.353978	3.428411
H	0.054928	–1.108183	4.666297
H	1.391941	–0.831790	3.570511
H	–0.145845	–2.999011	3.347056
H	–1.214101	–1.931912	2.456273
Complex			
Atom	X	Li–2–I Y	Z
Li	1.787676	0.977567	0.264279
C	2.204338	3.817667	0.594423
O	1.121539	2.912401	0.564098
O	3.381209	2.116616	–0.552065
C	3.064890	3.497933	–0.596771
O	3.096101	–0.481510	–1.630831
C	4.330433	0.209132	–1.628977
C	4.085335	1.688351	–1.702550
N	1.566623	–2.641146	–0.438773
C	1.959302	–2.580549	–1.835219
C	3.258815	–1.831515	–2.012871
C	0.116977	3.139360	1.535305
C	–0.769763	1.920886	1.521984
O	–0.031778	0.767768	1.886439
C	–0.165604	0.423187	3.256567
N	2.398745	–3.182699	0.444466
N	1.870819	–3.051551	1.620784
C	0.679850	–2.415674	1.515426
C	0.467091	–2.151276	0.181283
C	0.469261	–0.918070	3.543595
C	–0.119395	–2.085648	2.728765
I	–1.112250	–1.194944	–0.763457
I	–3.652867	0.948760	–2.205142
H	2.763980	3.698830	1.529373
H	1.851908	4.851356	0.526663
H	2.519503	3.717560	–1.520926
H	3.978192	4.100610	–0.576032
H	4.928421	–0.073910	–2.502141
H	4.901970	–0.046764	–0.728837
H	5.047234	2.208580	–1.765836
H	3.502220	1.925154	–2.599393
H	2.075180	–3.595542	–2.214098
H	1.156960	–2.096845	–2.388097
H	4.042419	–2.303575	–1.411488
H	3.552292	–1.890283	–3.067127
H	0.574210	3.278381	2.521679
H	–0.455595	4.037813	1.284303
H	–1.624445	2.066577	2.187186
H	–1.152883	1.756519	0.512139

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H	0.289273	1.196245	3.887632
H	−1.233709	0.378370	3.500990
H	0.317902	−1.106123	4.608448
H	1.549516	−0.867237	3.390063
H	−0.150580	−2.977471	3.356015
H	−1.149245	−1.861791	2.444210
Complex			
K−3−I			
Atom	X	Y	Z
K	2.496684	0.410960	1.008511
C	2.330727	3.834828	0.390292
O	1.325766	2.868991	0.612259
O	3.650616	2.231256	−0.770960
C	3.045695	3.501701	−0.890096
O	3.302984	−0.408066	−1.655954
C	4.508172	0.300409	−1.874261
C	4.196351	1.767791	−1.986821
N	1.670382	−2.416475	−0.338837
C	2.045403	−2.417672	−1.746132
C	3.391839	−1.776089	−1.981438
C	0.453929	3.204712	1.669476
C	−0.548024	2.101142	1.872983
O	0.087255	0.925896	2.351177
C	−0.763908	0.187371	3.215207
N	2.516454	−2.911093	0.563258
N	1.927990	−2.882647	1.718888
C	0.679733	−2.373695	1.581178
C	0.502368	−2.061114	0.249892
C	−0.121054	−1.104890	3.678039
C	−0.263361	−2.304768	2.733991
I	−1.107638	−1.137771	−0.683932
I	−3.809467	0.709217	−2.035759
H	3.033134	3.851520	1.233910
H	1.889703	4.833830	0.295921
H	2.327055	3.493099	−1.717687
H	3.799632	4.270941	−1.095497
H	4.977922	−0.023848	−2.809002
H	5.213103	0.108679	−1.055762
H	5.113192	2.317289	−2.231652
H	3.476582	1.919574	−2.799261
H	2.063119	−3.448545	−2.099124
H	1.273228	−1.879259	−2.291737
H	4.163325	−2.269547	−1.381570
H	3.646620	−1.900366	−3.039777
H	1.022658	3.365701	2.594373
H	−0.084002	4.130497	1.432472
H	−1.281930	2.453060	2.605071
H	−1.078134	1.882940	0.939163
H	−0.991875	0.812596	4.086623

H	–1.711471	–0.025170	2.704175
H	–0.610516	–1.373870	4.616360
H	0.929757	–0.927393	3.922063
H	–0.109132	–3.215233	3.315637
H	–1.288795	–2.344991	2.359827
Complex		Na–4–F	
Atom	X	Y	Z
Na	1.717419	0.586802	0.174173
C	2.296797	3.753557	0.657890
O	1.156718	2.928640	0.573497
O	3.510659	2.117438	–0.562891
C	3.150728	3.484548	–0.551291
O	3.148573	–0.431756	–1.697732
C	4.390424	0.246705	–1.745852
C	4.153666	1.731065	–1.758965
N	1.578373	–2.504456	–0.421521
C	1.955622	–2.499291	–1.823670
C	3.272732	–1.795456	–2.048725
C	0.182962	3.161371	1.570519
C	–0.784701	2.004268	1.527927
O	–0.146468	0.799214	1.908313
C	–0.375953	0.437158	3.258551
N	2.442699	–2.966267	0.481524
N	1.888090	–2.849608	1.646588
C	0.652183	–2.311171	1.505000
C	0.425778	–2.083391	0.161700
C	0.276061	–0.888981	3.575521
C	–0.206501	–2.057432	2.698497
I	–1.254262	–1.241225	–0.852496
F	–3.044547	–0.262359	–1.914267
H	2.850214	3.537458	1.580038
H	2.012940	4.811824	0.666234
H	2.586948	3.726239	–1.459899
H	4.045066	4.116839	–0.520307
H	4.932827	–0.020533	–2.659247
H	5.005473	–0.041491	–0.885286
H	5.116419	2.245764	–1.859202
H	3.529086	1.998013	–2.619643
H	2.032953	–3.526873	–2.179509
H	1.157909	–2.005040	–2.374729
H	4.057970	–2.268342	–1.451152
H	3.541074	–1.886017	–3.106949
H	0.658506	3.223801	2.557124
H	–0.339908	4.105207	1.378460
H	–1.643462	2.209973	2.172532
H	–1.152723	1.868294	0.508262
H	0.011100	1.214747	3.928784
H	–1.458353	0.362938	3.422521

H	0.047951	−1.101109	4.622292
H	1.362910	−0.799994	3.507123
H	−0.215290	−2.968408	3.299557
H	−1.234591	−1.881166	2.376191
Complex			
		Na–5–Cl	
Atom	X	Y	Z
Na	1.833410	0.608076	0.247024
C	2.351687	3.746958	0.696595
O	1.219800	2.912512	0.590952
O	3.571176	2.128728	−0.544995
C	3.214652	3.497374	−0.511351
O	3.135846	−0.411354	−1.702348
C	4.383038	0.257546	−1.778875
C	4.163509	1.744782	−1.768473
N	1.575631	−2.487695	−0.401269
C	1.931327	−2.477325	−1.811185
C	3.246579	−1.776024	−2.055110
C	0.216684	3.133085	1.560983
C	−0.748813	1.975738	1.471007
O	−0.133062	0.763014	1.868637
C	−0.379676	0.433315	3.225840
N	2.469677	−2.894285	0.496178
N	1.928902	−2.789959	1.668926
C	0.666199	−2.314790	1.546033
C	0.417874	−2.118467	0.204577
C	0.275960	−0.877416	3.594052
C	−0.181335	−2.077382	2.749003
I	−1.282564	−1.402134	−0.775685
Cl	−3.731083	−0.229400	−2.182721
H	2.898874	3.524273	1.620824
H	2.058985	4.802412	0.714606
H	2.655473	3.754922	−1.418102
H	4.110079	4.126699	−0.465511
H	4.894996	−0.004695	−2.710959
H	5.019955	−0.047408	−0.940370
H	5.128191	2.248034	−1.901319
H	3.509860	2.027393	−2.601953
H	1.999228	−3.504081	−2.170647
H	1.127046	−1.979623	−2.349331
H	4.040607	−2.253015	−1.473064
H	3.493791	−1.868407	−3.118087
H	0.661420	3.185802	2.562268
H	−0.302292	4.077716	1.363548
H	−1.634388	2.177249	2.079480
H	−1.073596	1.849849	0.435819
H	−0.007365	1.230600	3.880466
H	−1.463925	0.357426	3.374681
H	0.029175	−1.059926	4.642015

H	1.363400	−0.783671	3.543322
H	−0.140780	−2.977996	3.363724
H	−1.222078	−1.946952	2.446278
Complex		Na–6-I	
Atom	X	Y	Z
Na	1.366600	0.666655	−0.090510
C	2.334748	3.571816	0.717413
O	1.082305	2.947455	0.486430
O	3.563006	1.864785	−0.419703
C	3.225593	3.242633	−0.504141
O	3.211914	−0.318753	−2.131457
C	4.465762	−0.093684	−1.530394
C	4.609378	1.421967	−1.267089
N	1.448662	−2.040882	−0.647210
C	1.512506	−2.020988	−2.109574
C	2.952144	−1.650655	−2.541602
C	−0.004625	3.295609	1.325267
C	−1.048581	2.146625	1.229572
O	−0.487005	0.920556	1.664064
C	−0.804708	0.442587	2.960328
N	2.610434	−2.063256	0.037991
N	2.324294	−2.043859	1.286220
C	0.978500	−2.007017	1.438828
C	0.378087	−2.027492	0.196041
C	0.307926	−0.521748	3.440057
C	0.450459	−1.959565	2.842765
I	−1.659971	−2.038415	−0.367560
I	−4.790939	−1.937674	−1.262758
H	2.806080	3.163933	1.616791
H	2.654812	3.437211	−1.418185
H	4.533835	−0.644447	−0.586265
H	4.587765	1.949573	−2.224384
H	1.252114	−3.002895	−2.509306
H	3.639085	−2.360626	−2.079751
H	0.317797	3.417566	2.363384
H	−1.317925	2.009581	0.178340
H	−0.816550	1.272497	3.673363
H	1.251243	−0.013912	3.225066
H	1.248787	−2.407316	3.441624
C	−0.646042	4.538527	0.860747
N	−1.179545	5.474382	0.473658
C	2.234295	5.028676	0.892744
N	2.183940	6.158709	1.067967
C	4.403124	4.124516	−0.516050
N	5.307885	4.824479	−0.559109
C	5.918199	1.629770	−0.616936
N	6.927715	1.739141	−0.088447
C	5.573872	−0.530064	−2.398630

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N	6.413791	−0.899495	−3.083489
C	3.074805	−1.757007	−4.003000
N	3.167334	−1.835304	−5.141148
C	0.613275	−1.004691	−2.673998
N	0.023965	−0.139766	−3.138449
C	−0.706165	−2.829544	3.063375
N	−1.560606	−3.562468	3.274032
C	−2.147141	−0.164946	2.997981
N	−3.202226	−0.604126	3.064256
C	0.199143	−0.632724	4.896785
N	0.107642	−0.728337	6.034273
C	−2.265760	2.548820	1.944087
N	−3.194380	2.901513	2.512964
Complex		Na-7-I	
Atom	X	Y	Z
Na	2.083461	0.541211	0.931850
C	2.084362	3.805498	0.466255
O	1.098244	2.838721	0.733365
O	3.143560	2.072096	−0.726360
C	2.784915	3.413575	−0.835506
O	3.680127	−0.668748	−1.009491
C	4.672661	0.338471	−1.149600
C	3.981432	1.574822	−1.747789
N	1.586272	−2.345773	−0.608840
C	2.128433	−2.160406	−1.969421
C	3.622333	−1.785606	−1.883047
C	−0.021820	3.258004	1.440424
C	−0.923084	2.027781	1.584888
O	−0.129763	0.922014	2.025574
C	−0.197412	0.503347	3.360921
N	2.328783	−3.058520	0.236854
N	1.779994	−2.994638	1.401272
C	0.666472	−2.230545	1.330606
C	0.501065	−1.824361	0.024397
C	0.497786	−0.851553	3.461260
C	−0.120251	−1.966057	2.580420
I	−1.121034	−0.807474	−0.802039
I	−3.674023	1.392292	−1.855243
H	1.608585	4.783995	0.328454
H	3.678175	4.039047	−0.947478
H	4.977348	0.607466	−0.135920
H	4.733105	2.331314	−1.998406
H	2.027797	−3.104596	−2.503175
H	4.222611	−2.596851	−1.476923
H	−0.558893	4.042307	0.899697
H	−1.294608	1.747884	0.600185
H	−1.242799	0.425586	3.670076
H	0.373117	−1.185420	4.495041

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H	−1.133517	−1.662193	2.313077
O	0.515151	1.350510	4.227012
H	0.438801	2.268788	3.933796
O	1.874189	−0.684404	3.170448
H	2.194144	−0.013236	3.783488
O	−0.250223	−3.162145	3.323515
H	0.606286	−3.602155	3.319557
O	1.441224	−1.200026	−2.676987
H	1.733982	−0.314932	−2.408336
O	4.085777	−1.543774	−3.169390
H	3.455646	−0.971869	−3.627425
O	5.815340	−0.046424	−1.811641
H	5.567351	−0.398155	−2.677207
O	3.248616	1.198904	−2.870730
H	2.775740	1.974451	−3.195487
O	1.938289	3.555727	−1.943680
H	2.023841	4.440358	−2.307790
O	3.049031	3.834983	1.464183
H	2.628980	4.108319	2.285494
O	0.345192	3.731829	2.722435
H	0.059517	4.639792	2.847371
O	−2.012924	2.288314	2.380375
H	−1.756485	2.838624	3.128570
Complex			
Na−1−I + 127CH ₂ Cl ₂			
Atom	X	Y	Z
Na	2.019996	−1.119968	−0.338011
C	4.023975	1.153051	−1.396011
O	2.680975	1.116038	−0.948011
O	3.761996	−1.126952	−2.060011
C	4.141984	0.166052	−2.532011
O	1.766015	−3.190970	−2.032011
C	3.079017	−3.370958	−2.538011
C	3.630005	−2.074953	−3.093011
N	−0.030981	−3.616987	0.168989
C	−0.234976	−4.179989	−1.153011
C	1.097027	−4.422977	−1.840011
C	2.334966	2.122035	−0.007011
C	0.958969	1.775022	0.522989
O	0.996980	0.553022	1.260989
C	1.106978	0.742023	2.661989
N	0.834025	−4.195979	0.999989
N	0.847018	−3.492979	2.090989
C	−0.011992	−2.443987	1.988989
C	−0.602991	−2.524993	0.738989
C	1.088991	−0.598977	3.370989
C	−0.163001	−1.481988	3.125989
I	−2.078002	−1.398006	−0.202011
I	−4.879014	−0.029033	−1.945011

ARTICLE			Journal Name
C	6.672046	−6.430925	−0.913011
CI	8.091039	−5.727911	−1.688011
CI	6.412037	−5.550927	0.587989
C	5.369082	−10.330937	12.354989
CI	4.718067	−8.667943	12.301989
CI	5.552087	−10.881935	10.652989
C	−12.685029	1.587894	17.607989
CI	−11.238029	1.549908	18.630989
CI	−12.773016	0.187893	16.548989
C	1.526800	19.822027	6.376989
CI	1.047794	20.421023	7.911989
CI	0.571793	20.517018	5.077989
C	8.171111	−13.376910	3.514989
CI	8.577095	−11.754907	3.133989
CI	8.274119	−14.277910	2.096989
C	6.083101	−12.339930	−1.279011
CI	5.291088	−10.988937	−2.131011
CI	6.276097	−11.965928	0.450989
C	11.549049	−6.762879	1.439989
CI	12.615043	−6.196869	2.664989
CI	11.661042	−5.997878	−0.128011
C	0.199103	−12.525985	−10.237011
CI	1.252089	−11.107975	−10.170011
CI	0.280113	−13.643984	−8.899011
C	11.585029	−4.656879	7.121989
CI	11.681039	−5.696878	5.679989
CI	13.191027	−4.444863	7.847989
C	4.512129	−15.365945	−10.701011
CI	3.536141	−16.635954	−10.007011
CI	5.575124	−14.840935	−9.403011
C	−8.935125	11.780929	1.544989
CI	−8.734109	10.053931	1.405989
CI	−10.229128	12.159917	2.730989
C	5.116957	3.051061	−6.030011
CI	5.760968	1.901067	−4.788011
CI	5.241963	2.364062	−7.627011
C	−18.868985	−3.187164	2.247989
CI	−19.599997	−1.842170	3.015989
CI	−20.075975	−4.231175	1.460989
C	3.347066	−8.608956	2.556989
CI	3.289063	−8.248956	0.834989
CI	3.428081	−10.234955	2.928989
C	−4.728947	−7.196031	13.804989
CI	−6.182951	−6.771045	12.856989
CI	−3.531960	−5.868020	13.793989
C	2.854014	−3.057960	7.601989
CI	1.048013	−2.954977	7.255989
CI	3.608999	−1.464953	7.331989

Journal Name			ARTICLE
C	−0.057026	1.244012	11.108989
Cl	−1.293036	2.326001	10.442989
Cl	0.930979	0.678022	9.821989
C	−3.525971	−4.659020	5.426989
Cl	−2.643983	−3.388012	4.582989
Cl	−4.309978	−3.951027	6.801989
C	11.396977	0.901120	−13.385011
Cl	9.749979	0.635104	−12.920011
Cl	11.663965	2.229122	−14.509011
C	0.007909	8.152013	0.955989
Cl	0.809919	7.073021	−0.210011
Cl	1.128897	9.409024	1.527989
C	3.291165	−19.138956	−6.914011
Cl	1.766168	−19.530970	−7.850011
Cl	4.615168	−19.496944	−7.995011
C	6.642045	−6.375925	5.493989
Cl	7.442033	−5.062917	4.668989
Cl	7.149046	−6.494920	7.097989
C	−13.010961	−5.734109	−3.174011
Cl	−12.515945	−7.416104	−3.369011
Cl	−14.397964	−5.445122	−4.227011
C	−0.130116	10.800012	4.805989
Cl	−1.275119	11.178001	3.498989
Cl	−0.857108	9.958005	6.099989
C	−5.258933	−8.731036	3.910989
Cl	−5.581940	−7.920039	5.415989
Cl	−4.285942	−7.727027	2.877989
C	−2.647071	6.031988	6.138989
Cl	−1.511079	6.831999	7.278989
Cl	−3.783082	7.185978	5.444989
C	4.535145	−17.046945	0.473989
Cl	4.130149	−17.466948	2.146989
Cl	5.513132	−15.682935	0.218989
C	0.338952	3.517016	−4.748011
Cl	−1.319051	3.909001	−5.074011
Cl	1.270939	4.966025	−4.633011
C	−8.739921	−10.030069	−2.730011
Cl	−7.243916	−10.532055	−3.553011
Cl	−8.676915	−10.687068	−1.093011
C	−3.839074	6.356977	−3.044011
Cl	−2.211074	6.336992	−2.283011
Cl	−4.854086	7.603968	−2.393011
C	−16.292030	1.638861	−6.517011
Cl	−15.892041	2.780864	−7.798011
Cl	−17.235038	2.443852	−5.263011
C	6.855992	−0.657923	5.001989
Cl	5.760979	0.656067	5.389989
Cl	7.209000	−1.610919	6.433989

ARTICLE			Journal Name
C	-9.445042	2.939925	-11.082011
CI	-9.900057	4.518920	-10.424011
CI	-9.059031	1.766928	-9.815011
C	3.163074	-9.475957	-6.785011
CI	3.527090	-11.224954	-7.048011
CI	4.618065	-8.502944	-6.210011
C	-4.419895	-12.751028	1.195989
CI	-3.194883	-14.069017	1.136989
CI	-3.851911	-11.120023	1.550989
C	-12.227996	-1.974101	8.589989
CI	-12.302011	-0.437102	7.683989
CI	-10.683989	-2.758087	8.409989
C	-16.577951	-6.807142	-0.394011
CI	-15.262942	-7.749130	-1.178011
CI	-18.200949	-7.035157	-1.092011
C	-4.972913	-10.840034	-7.224011
CI	-4.965898	-12.456033	-6.592011
CI	-4.031914	-10.711025	-8.711011
C	-16.771992	-2.445144	-6.789011
CI	-18.267993	-2.269158	-7.752011
CI	-15.444986	-3.042132	-7.773011
C	6.687947	4.096076	-16.895011
CI	6.086952	3.561070	-15.365011
CI	8.387942	4.631092	-16.766011
C	-10.852958	-6.033089	-7.673011
CI	-10.448962	-5.579085	-9.301011
CI	-12.225968	-4.977101	-7.063011
C	7.294952	3.555081	-11.929011
CI	8.123957	3.080089	-10.478011
CI	8.116940	4.883089	-12.641011
C	-20.756963	-5.503181	-4.292011
CI	-21.049970	-4.784184	-5.898011
CI	-20.578975	-4.195180	-3.042011
C	-4.727053	4.052969	2.586989
CI	-5.322057	4.574963	0.999989
CI	-2.976055	4.363985	2.653989
C	-12.934057	4.568892	-6.087011
CI	-11.464062	5.095906	-7.004011
CI	-14.262069	5.759880	-5.974011
C	-1.866988	-2.883004	-8.816011
CI	-2.862998	-1.798014	-9.778011
CI	-1.055978	-3.942997	-9.905011
C	-6.180988	-2.806045	-9.529011
CI	-6.346992	-2.367046	-7.768011
CI	-6.707000	-1.537050	-10.568011
C	2.201952	3.557034	7.496989
CI	1.530943	4.537027	8.851989
CI	4.014952	3.537051	7.325989

Journal Name			ARTICLE
C	12.579928	6.080131	−0.769011
Cl	13.383940	4.877138	−1.823011
Cl	13.641925	6.399141	0.584989
C	9.167913	7.694099	2.880989
Cl	8.547898	9.337093	2.680989
Cl	10.948914	7.579116	2.505989
C	0.013916	7.460013	11.583989
Cl	1.046912	7.805023	10.237989
Cl	0.907921	6.843022	12.960989
C	2.848917	7.315040	6.645989
Cl	1.756919	7.106029	5.315989
Cl	2.556902	8.900037	7.268989
C	1.403978	0.739026	−9.986011
Cl	−0.075026	1.207012	−9.084011
Cl	0.989984	0.107022	−11.615011
C	−10.915960	−5.811089	4.033989
Cl	−12.429954	−6.477103	4.508989
Cl	−9.660949	−6.959077	4.229989
C	6.175994	−0.941929	−12.033011
Cl	6.302994	−0.925928	−10.278011
Cl	4.508991	−0.651945	−12.453011
C	−8.795050	3.785931	−4.463011
Cl	−8.229043	3.063936	−2.954011
Cl	−8.188044	3.097936	−5.899011
C	−10.405064	5.244916	9.962989
Cl	−10.943074	6.394911	8.767989
Cl	−11.592052	4.024905	10.105989
C	−10.895007	−0.827089	−4.914011
Cl	−11.781003	−1.284097	−6.370011
Cl	−10.671023	0.896913	−4.748011
C	4.095022	−3.904949	−8.814011
Cl	3.418029	−4.611955	−7.350011
Cl	2.934019	−3.599960	−10.135011
C	10.074987	−0.123893	9.457989
Cl	10.121974	1.180108	8.289989
Cl	11.051984	0.187116	10.926989
C	−0.875128	12.125005	−4.444011
Cl	−0.686138	13.224007	−3.149011
Cl	−2.485122	11.459990	−4.461011
C	−3.581023	0.931980	−12.440011
Cl	−2.024028	1.467994	−12.767011
Cl	−4.090012	−0.237025	−13.557011
C	−1.569128	12.130998	10.198989
Cl	−2.377138	13.147991	8.988989
Cl	0.073868	12.535014	10.587989
C	9.141922	6.822099	−8.619011
Cl	9.714909	8.124104	−7.649011
Cl	10.402930	5.893110	−9.432011

ARTICLE			Journal Name
C	15.591972	1.402159	8.225989
CI	16.037988	−0.284837	8.665989
CI	13.941971	1.588144	8.208989
C	−9.575956	−6.271077	8.436989
CI	−9.789956	−6.224079	10.163989
CI	−9.753941	−7.869078	7.762989
C	5.404028	−4.556936	10.777989
CI	4.763041	−5.890942	9.720989
CI	4.174016	−3.307948	11.286989
C	−6.607008	−0.673049	6.665989
CI	−6.171004	−1.117045	5.079989
CI	−5.085013	−0.182035	7.387989
C	−7.399119	11.096944	−3.884011
CI	−6.315128	12.146954	−2.912011
CI	−8.785126	11.945931	−4.577011
C	5.261914	7.635062	−0.831011
CI	4.800914	7.667058	0.872989
CI	5.435899	9.189064	−1.453011
C	−9.696020	0.580922	12.315989
CI	−10.444011	−0.378085	10.974989
CI	−10.879029	1.521911	13.151989
C	7.489908	8.309083	8.623989
CI	7.921909	8.160087	6.931989
CI	7.099922	6.792079	9.402989
C	17.411946	4.222176	0.821989
CI	17.272940	4.822175	−0.852011
CI	19.015952	3.548191	1.146989
C	−0.734911	−11.081994	6.218989
CI	−1.483907	−11.478001	7.741989
CI	−1.213927	−9.356998	5.944989
C	−2.085076	6.588994	−12.953011
CI	−2.198066	5.434992	−11.581011
CI	−3.331088	7.806982	−12.898011
C	−5.182135	12.831965	−8.695011
CI	−3.522130	12.318980	−9.037011
CI	−5.943127	11.990957	−7.286011
C	1.323068	−8.878975	8.406989
CI	2.608067	−8.726963	7.229989
CI	1.165054	−7.347976	9.385989
C	−5.084957	−6.197035	−5.601011
CI	−5.556942	−7.761039	−4.924011
CI	−5.723970	−4.820041	−4.726011
C	−9.159097	8.787927	−8.437011
CI	−7.628089	7.951942	−8.510011
CI	−9.716098	8.939922	−6.801011
C	−3.520105	9.642980	1.038989
CI	−3.888088	7.877977	0.991989
CI	−4.647112	10.429970	2.151989

Journal Name			ARTICLE
C	−4.420151	14.552972	0.893989
Cl	−3.540154	14.899980	−0.550011
Cl	−3.446146	13.990981	2.156989
C	−7.918088	7.850939	−12.477011
Cl	−7.335104	9.518944	−12.360011
Cl	−9.525089	7.910924	−13.128011
C	−15.744998	−1.788134	4.849989
Cl	−14.955983	−3.384127	4.794989
Cl	−14.570011	−0.438123	4.852989
C	9.329113	−13.681900	9.969989
Cl	10.184118	−14.146892	11.431989
Cl	9.824122	−14.600895	8.618989
C	−9.437025	1.147925	4.530989
Cl	−9.772011	−0.409078	5.204989
Cl	−10.700036	2.245913	4.965989
C	8.718079	−10.053905	−5.254011
Cl	7.686092	−11.416915	−5.367011
Cl	8.273073	−9.334910	−3.674011
C	−4.060059	4.766975	−8.556011
Cl	−4.859064	5.250968	−7.012011
Cl	−5.381056	4.406963	−9.658011
C	14.051949	3.879145	−7.083011
Cl	12.711957	3.021132	−7.707011
Cl	13.689934	5.466141	−6.461011
C	11.001084	−10.501884	0.281989
Cl	12.469085	−10.596870	1.148989
Cl	10.460099	−12.094889	−0.174011
C	6.006847	14.817069	7.559989
Cl	4.958858	13.629059	8.357989
Cl	7.640847	14.770085	8.299989
C	−5.309055	4.297963	12.872989
Cl	−4.825046	3.396968	11.453989
Cl	−5.419045	3.209962	14.284989
C	7.708964	2.312085	0.176989
Cl	9.065969	1.796098	−0.786011
Cl	6.933976	1.043078	1.094989
C	−5.661156	15.079960	−5.018011
Cl	−5.561167	16.252961	−3.719011
Cl	−4.061153	14.819975	−5.758011
C	0.918927	6.234022	−9.353011
Cl	2.592928	6.172037	−8.727011
Cl	−0.092063	5.143012	−8.582011
C	15.253927	6.229156	5.423989
Cl	15.600913	7.777159	4.783989
Cl	16.738936	5.243170	5.452989
C	1.073855	13.969023	0.904989
Cl	1.566843	15.188028	−0.230011
Cl	2.524863	13.064037	1.481989

ARTICLE			Journal Name
C	10.797030	−4.780886	−5.070011
CI	12.236025	−4.209872	−5.906011
CI	10.169018	−3.517892	−3.941011
C	14.852018	−3.490848	−1.627011
CI	16.216010	−2.655835	−2.366011
CI	14.297010	−2.657853	−0.175011
C	1.896117	−14.058969	1.492989
CI	2.531112	−13.493963	−0.065011
CI	0.329110	−13.261984	1.858989
C	13.058991	−0.567865	4.612989
CI	13.726001	−1.641858	5.788989
CI	11.838981	0.453124	5.452989
C	13.933960	2.748143	1.499989
CI	14.990966	2.100153	2.813989
CI	12.244962	2.536128	1.910989
C	6.597897	9.470075	−6.237011
CI	5.600908	8.256065	−7.065011
CI	7.125902	8.878080	−4.665011
C	6.632862	13.208075	1.494989
CI	6.189870	12.359071	−0.035011
CI	6.109846	14.893070	1.419989
C	9.797981	0.419105	−6.624011
CI	9.551977	0.841102	−4.907011
CI	8.246979	0.709090	−7.432011
C	−15.883002	−1.303136	−2.057011
CI	−15.488002	−1.332132	−0.358011
CI	−14.533998	−1.789123	−3.067011
C	−12.583931	−8.938105	1.201989
CI	−13.874935	−8.471117	2.177989
CI	−11.850944	−7.596098	0.429989
C	5.703962	2.506066	10.665989
CI	6.710962	2.468076	9.231989
CI	4.625974	1.167056	10.621989
C	−1.603174	16.997998	5.350989
CI	−1.054168	16.424003	3.791989
CI	−1.492162	15.696999	6.560989
C	−5.415880	−14.362038	−2.908011
CI	−6.048881	−14.309044	−1.324011
CI	−3.918889	−13.454024	−2.849011
C	3.068044	−6.298958	−13.098011
CI	1.819046	−6.515970	−11.900011
CI	4.637049	−6.817944	−12.535011
C	10.038934	5.484107	−3.676011
CI	10.023945	4.311107	−4.956011
CI	8.349931	5.783091	−3.090011
C	9.522058	−7.792898	11.787989
CI	9.937049	−6.746894	13.167989
CI	8.117053	−7.255911	10.813989

Journal Name			ARTICLE
C	-2.260100	9.135992	-7.896011
Cl	-1.073093	8.377003	-6.831011
Cl	-3.900099	9.028977	-7.332011
C	14.463981	0.422148	-3.998011
Cl	13.312986	-0.116862	-2.738011
Cl	14.873966	2.070152	-3.852011
C	-11.817992	-2.420098	0.150989
Cl	-12.394977	-4.070103	0.251989
Cl	-10.567993	-2.311086	-1.123011
C	8.879009	-2.507904	-0.229011
Cl	8.242008	-2.459910	1.389989
Cl	10.201998	-1.394891	-0.487011
C	-8.353954	-6.426065	-0.793011
Cl	-7.502961	-5.699057	-2.074011
Cl	-9.297965	-5.293074	0.000989
C	-5.762993	-2.339041	11.122989
Cl	-7.499992	-2.398057	10.940989
Cl	-5.407986	-3.062038	12.671989
C	-5.711094	8.506960	9.882989
Cl	-7.409090	8.079944	9.667989
Cl	-4.666081	7.070969	10.051989
C	-7.310009	-0.613055	15.996989
Cl	-6.176009	-0.571045	17.375989
Cl	-6.633014	-0.031049	14.422989
C	11.111894	9.716117	-0.643011
Cl	12.304896	9.510128	-1.916011
Cl	9.567902	8.866103	-0.973011
C	-0.704984	-3.305994	12.473989
Cl	-0.135970	-4.793988	13.268989
Cl	-0.000986	-3.051987	10.770989
C	2.007957	2.984032	-14.755011
Cl	1.119953	3.431024	-13.334011
Cl	3.135969	1.776042	-14.370011
C	-3.010936	-8.363015	-1.912011
Cl	-4.313931	-8.956027	-0.988011
Cl	-3.295952	-6.666018	-2.321011
C	-12.105034	2.047900	-0.132011
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H	3.705019	−3.639952	−1.701011
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H	−0.693966	−5.145993	−1.020011
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H	3.032966	2.052041	0.810989
H	0.327970	1.598016	−0.331011
H	0.683961	2.556019	1.210989
H	0.231973	1.291015	2.971989
H	2.076974	1.170032	2.849989
H	1.078989	−0.366977	4.420989
H	1.923996	−1.150969	2.974989
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H	6.920055	−7.438922	−0.652011
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H	4.624088	−10.949944	12.810989
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H	−6.278160	15.516954	−5.775011
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H	−16.082012	−0.279138	−2.299011
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H	−8.089015	0.075937	16.245989
H	−7.538999	−1.647058	15.844989
H	10.875885	10.759115	−0.627011
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H	−11.797043	3.067903	−0.033011
H	17.495990	−0.471823	1.016989
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Receptor	1–5		
Atom	X	Y	Z
C	2.316801	3.691657	0.648893
O	1.115935	2.965648	0.625351
O	3.478741	2.108206	−0.693182
C	3.058033	3.448221	−0.638893
O	3.197681	−0.495941	−1.890772
C	4.365860	0.289547	−1.948445
C	4.001769	1.749572	−1.945633
N	1.706174	−2.564086	−0.387926
C	2.189053	−2.644748	−1.757299
C	3.468929	−1.869041	−1.970934
C	0.312121	3.151732	1.762479
C	−0.795388	2.122602	1.732789
O	−0.321173	0.824706	2.006849

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C	−0.442148	0.443263	3.357334
N	2.414020	−3.138513	0.577161
N	1.776057	−2.978843	1.693843
C	0.629074	−2.293729	1.471661
C	0.577956	−2.018307	0.125042
C	0.205631	−0.909375	3.559467
C	−0.310637	−1.991156	2.589541
I	−0.857052	−1.047702	−0.980481
H	2.935283	3.382526	1.502247
H	2.120586	4.768687	0.745583
H	2.395750	3.674047	−1.485218
H	3.920441	4.126956	−0.694687
H	4.925487	0.070568	−2.867778
H	5.016448	0.064528	−1.093638
H	4.903575	2.336058	−2.171400
H	3.266488	1.945493	−2.737558
H	2.357244	−3.695745	−1.988829
H	1.405959	−2.268943	−2.412463
H	4.210774	−2.165602	−1.219638
H	3.868107	−2.129815	−2.960229
H	0.906327	3.035083	2.679246
H	−0.117921	4.163585	1.768308
H	−1.581945	2.406064	2.441591
H	−1.232363	2.103447	0.731284
H	0.031959	1.182213	4.016368
H	−1.507268	0.394829	3.627730
H	0.009043	−1.212271	4.589634
H	1.288645	−0.816499	3.460325
H	−0.468263	−2.921206	3.137758
H	−1.279039	−1.696705	2.181719
Receptor		6	
Atom	X	Y	Z
C	2.446484	2.925326	1.087028
O	1.294989	2.519745	0.383465
O	3.881404	1.683838	−0.338931
C	3.606984	2.994934	0.072007
O	3.113012	−0.132588	−2.362600
C	4.442433	0.063930	−1.962088
C	4.569714	1.542262	−1.554172
N	1.446670	−1.686771	−0.403697
C	1.323884	−1.653533	−1.851886
C	2.705547	−1.467740	−2.510495
C	0.039972	2.902296	0.886112
C	−0.922450	1.715584	0.650439
O	−0.539475	0.607643	1.421961
C	−0.908085	0.541835	2.777624
N	2.565191	−1.259123	0.189335
N	2.359991	−1.267847	1.456284

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C	1.099808	−1.689338	1.708565
C	0.492362	−1.980834	0.513354
C	0.232697	−0.170821	3.544033
C	0.615444	−1.626989	3.125720
I	−1.387881	−2.642351	0.025278
H	2.700366	2.189080	1.856701
H	3.293149	3.623548	−0.767511
H	4.682423	−0.552988	−1.089642
H	4.126373	2.164412	−2.339433
H	0.898653	−2.600662	−2.190089
H	3.395939	−2.168134	−2.034464
H	0.070935	3.122183	1.957942
H	−0.816936	1.397027	−0.389048
H	−1.009671	1.536813	3.221965
H	1.124933	0.428671	3.354807
H	1.478733	−1.878518	3.748074
C	−0.435481	4.111831	0.188658
N	−0.789383	5.044989	−0.372839
C	2.285797	4.234135	1.743519
N	2.130038	5.242006	2.264578
C	4.780067	3.621794	0.718793
N	5.677416	4.105406	1.240355
C	5.998419	1.899915	−1.431929
N	7.107955	2.169652	−1.346438
C	5.374498	−0.271159	−3.056546
N	6.067730	−0.570625	−3.917549
C	2.611159	−1.810472	−3.941873
N	2.528206	−2.071611	−5.053427
C	0.420285	−0.561865	−2.251326
N	−0.279141	0.297546	−2.538777
C	−0.402671	−2.623940	3.458877
N	−1.162646	−3.423766	3.766708
C	−2.213330	−0.130433	2.939064
N	−3.231702	−0.637167	3.070172
C	−0.041162	−0.112778	4.979340
N	−0.264599	−0.073738	6.102009
C	−2.321938	2.117078	0.860572
N	−3.408120	2.431255	1.041954
Receptor			7
Atom	X	Y	Z
C	2.395185	3.460803	0.367224
O	1.391232	2.490921	0.468700
O	3.474246	1.945776	−1.087131
C	3.139423	3.286812	−0.955856
O	4.142287	−0.635199	−1.241803
C	5.018578	0.313541	−1.794181
C	4.304069	1.623791	−2.173817
N	1.656704	−1.766228	−0.135076

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C	1.847941	−1.297694	−1.510897
C	3.296935	−1.463698	−2.009776
C	0.244761	2.910213	1.147484
C	−0.715864	1.718254	1.210165
O	−0.152990	0.724582	2.047963
C	−0.892894	0.283843	3.147251
N	2.669006	−1.987866	0.703379
N	2.171012	−2.180772	1.879600
C	0.824398	−2.074412	1.827117
C	0.476606	−1.838682	0.526674
C	−0.133217	−0.840628	3.844295
C	0.003874	−2.166101	3.069049
I	−1.384994	−1.719715	−0.334379
H	1.935906	4.459500	0.355075
H	4.042962	3.906969	−0.930226
H	5.676287	0.568643	−0.963072
H	5.061906	2.406594	−2.299250
H	1.218995	−1.918666	−2.149345
H	3.623576	−2.496002	−1.877545
H	−0.250632	3.712747	0.588370
H	−0.806561	1.303280	0.203884
H	−1.881259	−0.071917	2.845160
H	−0.741982	−1.089145	4.721807
H	−1.005375	−2.501693	2.812830
O	−1.130815	1.328490	4.058900
H	−0.267543	1.644525	4.351255
O	1.110789	−0.322700	4.249272
H	1.501089	−0.936747	4.875155
O	0.564814	−3.121152	3.953907
H	1.497932	−3.208798	3.731525
O	1.397039	0.003369	−1.642307
H	1.992778	0.613325	−1.174199
O	3.315390	−1.205610	−3.373637
H	2.996701	−0.296076	−3.515063
O	5.829451	−0.161747	−2.813293
H	5.261058	−0.464203	−3.531444
O	3.570644	1.473828	−3.356335
H	2.991594	2.242921	−3.433169
O	2.327183	3.653535	−2.048536
H	2.490789	4.571434	−2.277316
O	3.325961	3.349981	1.394143
H	2.833880	3.365662	2.222127
O	0.563759	3.360682	2.440679
H	0.305311	4.278979	2.534760
O	−1.983231	2.129741	1.591548
H	−1.933229	2.415374	2.514698

ARTICLE

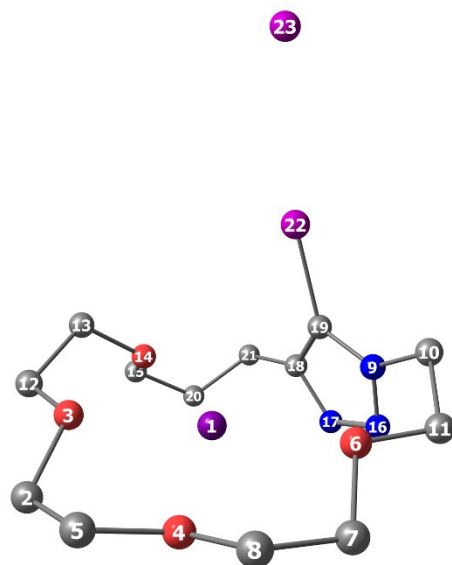


Figure S1. Atoms numeration to structures Na-1-I and Na-1-I + 127 CH₂Cl₂. Atoms color: Sodium (purple); carbon (gray); oxygen (red); nitrogen (blue); and iodine (pink).

Table S2. Bond lengths (r / Å) and angles ($\angle$ / °) to structures Na-1-I and Na-1-I + 127 CH₂Cl₂.

Geometric Parameter	1	1 + 127CH ₂ Cl ₂	Absolute Deviation ^[a]
r[C(2)–O(3)]	1.410	1.416	0.006
r[C(2)–C(5)]	1.505	1.509	0.004
r[O(3)–C(12)]	1.413	1.420	0.007
r[O(4)–C(5)]	1.414	1.428	0.014
r[O(4)–C(8)]	1.412	1.408	0.004
r[O(6)–C(7)]	1.417	1.419	0.002
r[O(6)–C(11)]	1.413	1.415	0.002
r[C(7)–C(8)]	1.503	1.514	0.011
r[N(9)–C(10)]	1.455	1.451	0.004
r[N(9)–N(16)]	1.329	1.332	0.003
r[N(9)–C(19)]	1.357	1.358	0.001
r[C(10)–C(11)]	1.511	1.518	0.007
r[C(12)–C(13)]	1.509	1.515	0.006
r[C(13)–O(14)]	1.418	1.428	0.010
r[O(14)–C(15)]	1.418	1.418	0.000
r[C(15)–C(20)]	1.511	1.517	0.006
r[N(16)–N(17)]	1.296	1.298	0.002
r[N(17)–C(18)]	1.355	1.360	0.005
r[C(18)–C(19)]	1.377	1.385	0.008
r[C(18)–C(21)]	1.491	1.497	0.006
r[C(19)–I(22)]	2.076	2.081	0.005
r[C(20)–C(21)]	1.537	1.552	0.015
$\angle$ [O(3)–C(2)–C(5)]	107.5	107.2	0.3
$\angle$ [C(2)–O(3)–C(12)]	115.1	115.0	0.1
$\angle$ [C(2)–C(5)–O(4)]	108.9	108.8	0.1
$\angle$ [O(3)–C(12)–C(13)]	107.0	106.9	0.1
$\angle$ [C(5)–O(4)–C(8)]	112.9	113.1	0.2
$\angle$ [O(4)–C(8)–C(7)]	109.7	110.0	0.3
$\angle$ [C(7)–O(6)–C(11)]	112.3	112.1	0.2
$\angle$ [O(6)–C(7)–C(8)]	109.6	111.0	1.4
$\angle$ [O(6)–C(11)–C(10)]	109.6	109.7	0.1
$\angle$ [C(10)–N(9)–N(16)]	119.4	119.4	0.0
$\angle$ [C(10)–N(9)–C(19)]	130.1	129.4	0.7
$\angle$ [N(9)–C(10)–C(11)]	111.7	110.5	1.2
$\angle$ [N(16)–N(9)–C(19)]	110.5	111.2	0.7
$\angle$ [N(9)–N(16)–N(17)]	107.9	107.2	0.7
$\angle$ [N(9)–C(19)–C(18)]	104.3	104.2	0.1
$\angle$ [N(9)–C(19)–I(22)]	125.4	123.0	2.4
$\angle$ [C(12)–C(13)–O(14)]	111.1	110.6	0.5
$\angle$ [C(12)–O(14)–C(15)]	113.3	113.5	0.2
$\angle$ [O(14)–C(15)–C(20)]	110.6	110.1	0.5
$\angle$ [C(15)–C(20)–C(21)]	114.1	116.0	1.9
$\angle$ [N(16)–N(17)–C(18)]	109.6	110.4	0.8
$\angle$ [N(17)–C(18)–C(19)]	107.6	107.0	0.6
$\angle$ [N(17)–C(18)–C(21)]	120.7	120.2	0.5
$\angle$ [C(19)–C(18)–C(21)]	131.7	132.8	1.1
$\angle$ [C(18)–C(19)–I(22)]	130.3	132.8	2.5
$\angle$ [C(18)–C(21)–C(20)]	113.5	113.8	0.3

^[a] | Result(1 + 127CH₂Cl₂) – Result(1) |.

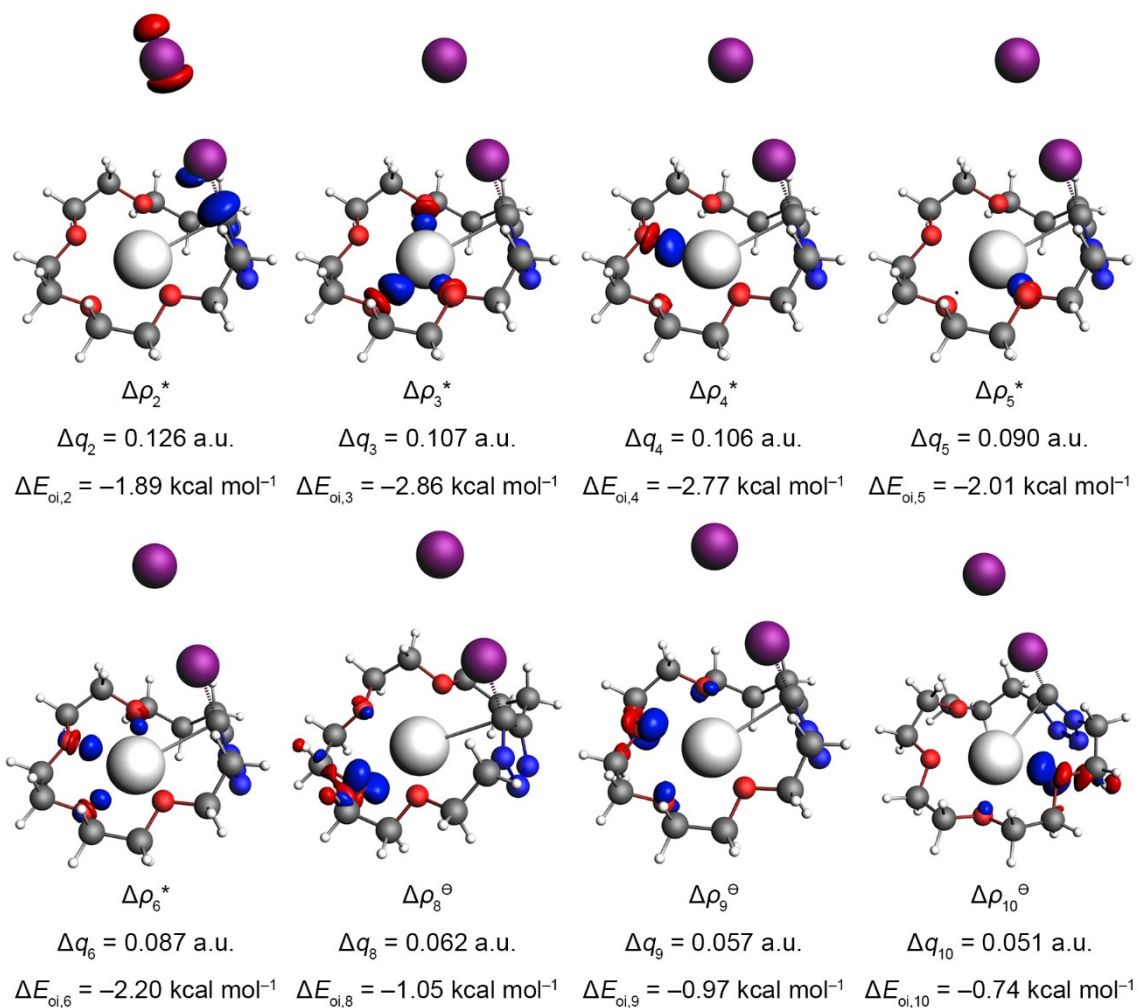


Figure S2. Selected density flow channels: $\Delta\rho_{2-6}$ and $8-10$ for $\text{Na}^+\cdots\text{1-I}^-$, with their respective energy, $\Delta E_{oi,k}$, and charge transfer estimation, Δq_k . Red and blue regions indicate the electronic density outflow and inflow, respectively. The isovalues used to represent these surfaces are equal to: $*$ = 0.0010 and $\ominus$ = 0.0005 a.u.

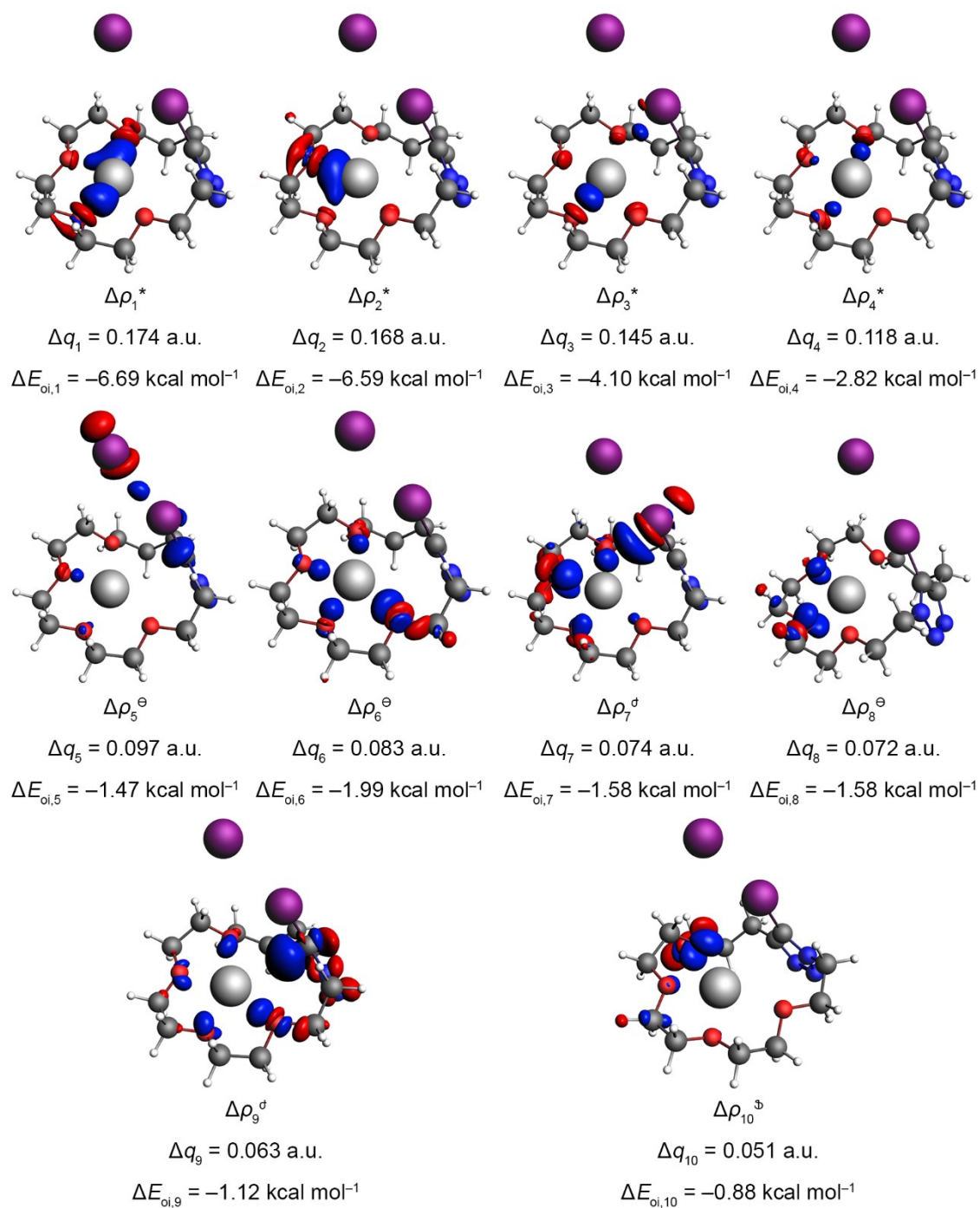


Figure S3. Selected density flow channels: $\Delta\rho_{1-10}$ for $\text{Li}^+\cdots\text{2-I}^-$, with their respective energy, $\Delta E_{\text{oi},k}$, and charge transfer estimation, Δq_k . Red and blue regions indicate the electronic density outflow and inflow, respectively. The isovalues used to represent these surfaces are equal to: $*$ = 0.0010; $\ominus$ = 0.0005; $\boxplus$ = 0.0003 and $\boxminus$ = 0.0002 a.u.

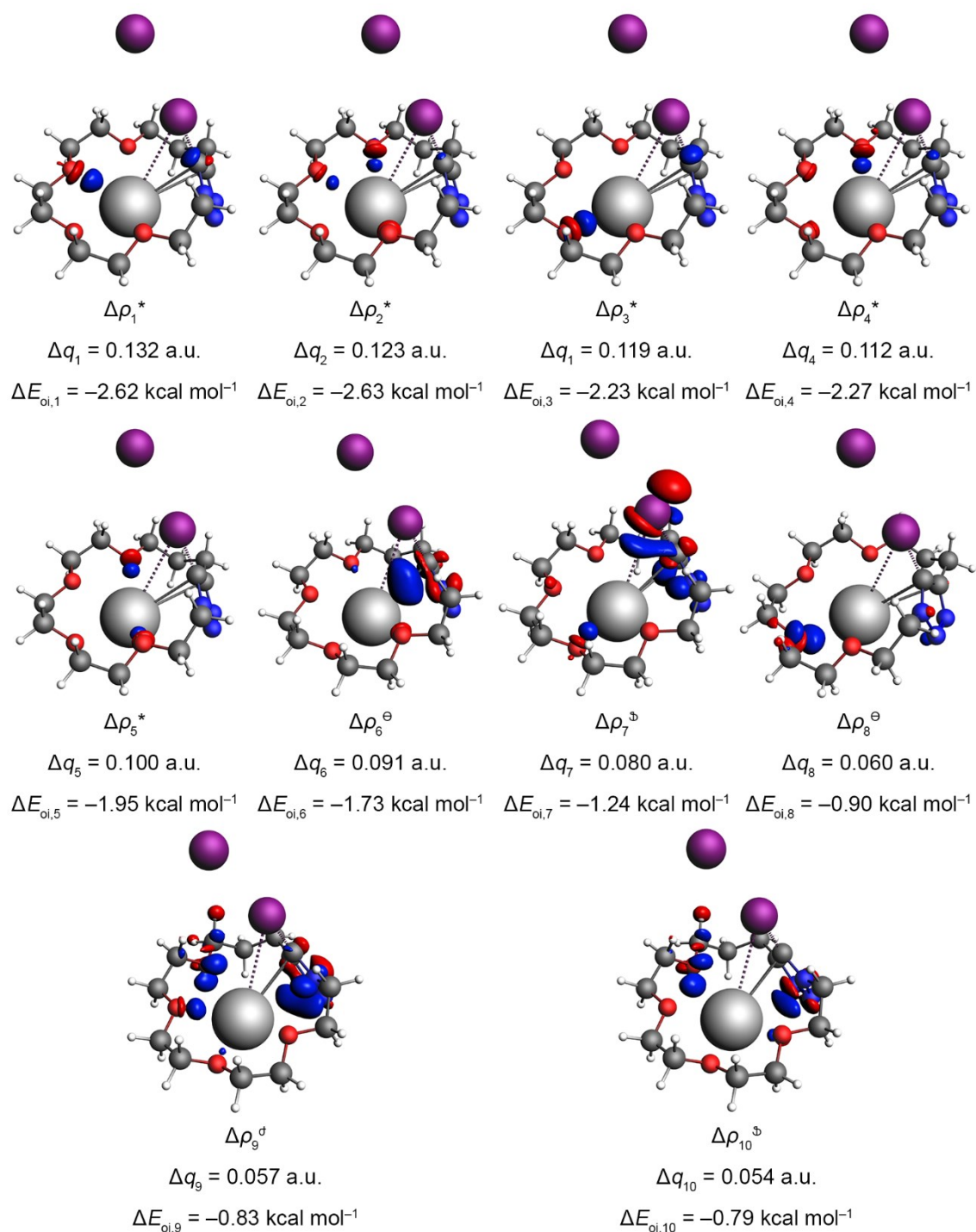


Figure S4. Selected density deformation channels surface plots: $\Delta\rho_{1-10}$ for $K^+ \cdots 3-I^-$, with their respective energy, $\Delta E_{oi,k}$, and charge transfer estimation, Δq_k . Red and blue regions indicate the electronic density outflow and inflow, respectively. The isovalues used to represent these surfaces are equal to: $*$ = 0.0010; $\ominus$ = 0.0005; δ = 0.0003 and $\square$ = 0.0002 a.u.

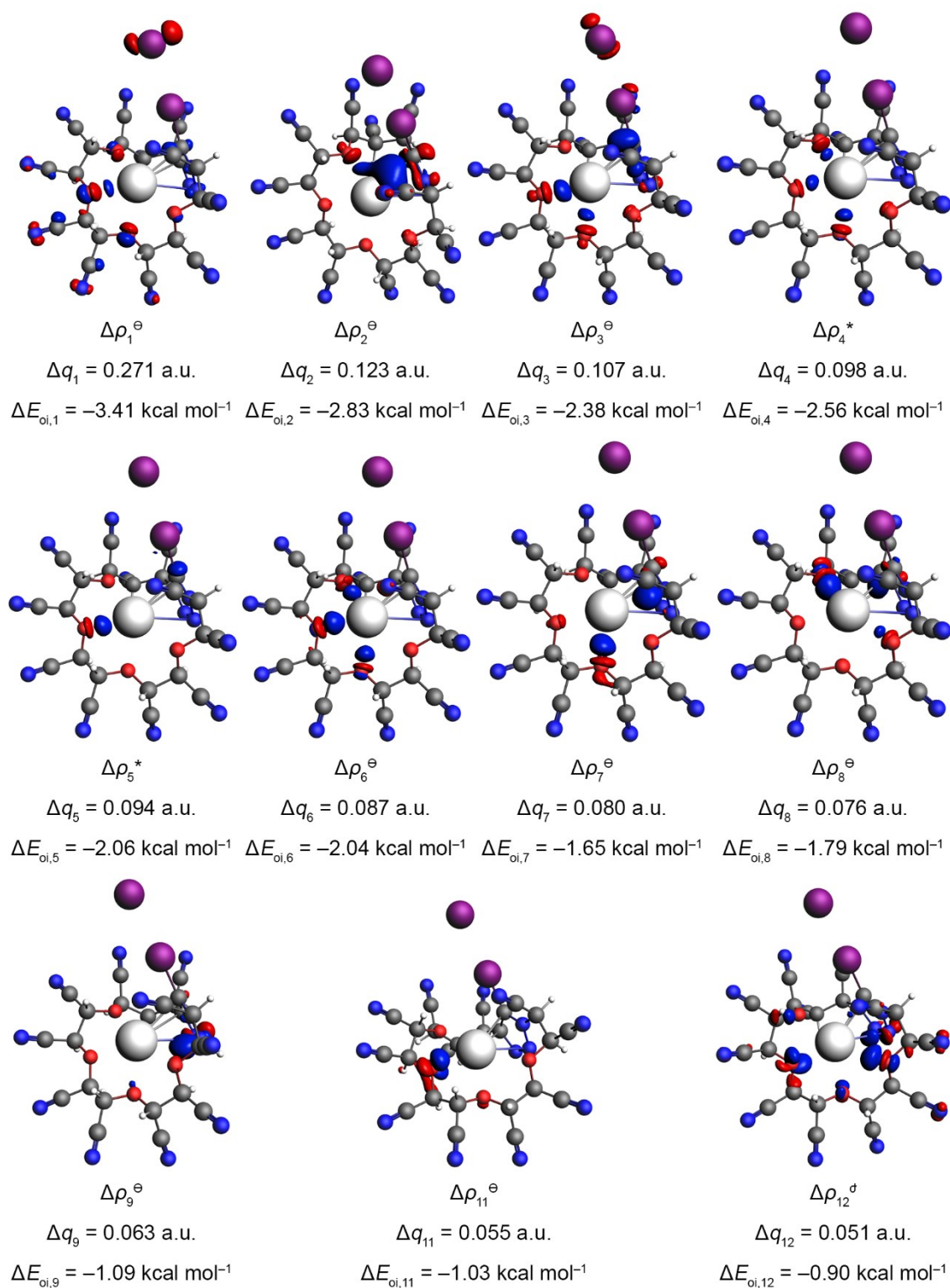


Figure S5. Selected density flow channels: $\Delta \rho_{1-9,11}$ and 12 for $\text{Na}^+ \cdots 6\text{-I}^-$, with their respective energy, $\Delta E_{\text{oi},k}$ and charge transfer estimation, Δq_k . Red and blue regions indicate the electronic density outflow and inflow, respectively. The isovalues used to represent these surfaces are equal to: $*$ = 0.0010; $\ominus$ = 0.0005; $\boxminus$ = 0.0003 and $\boxplus$ = 0.0002 a.u.

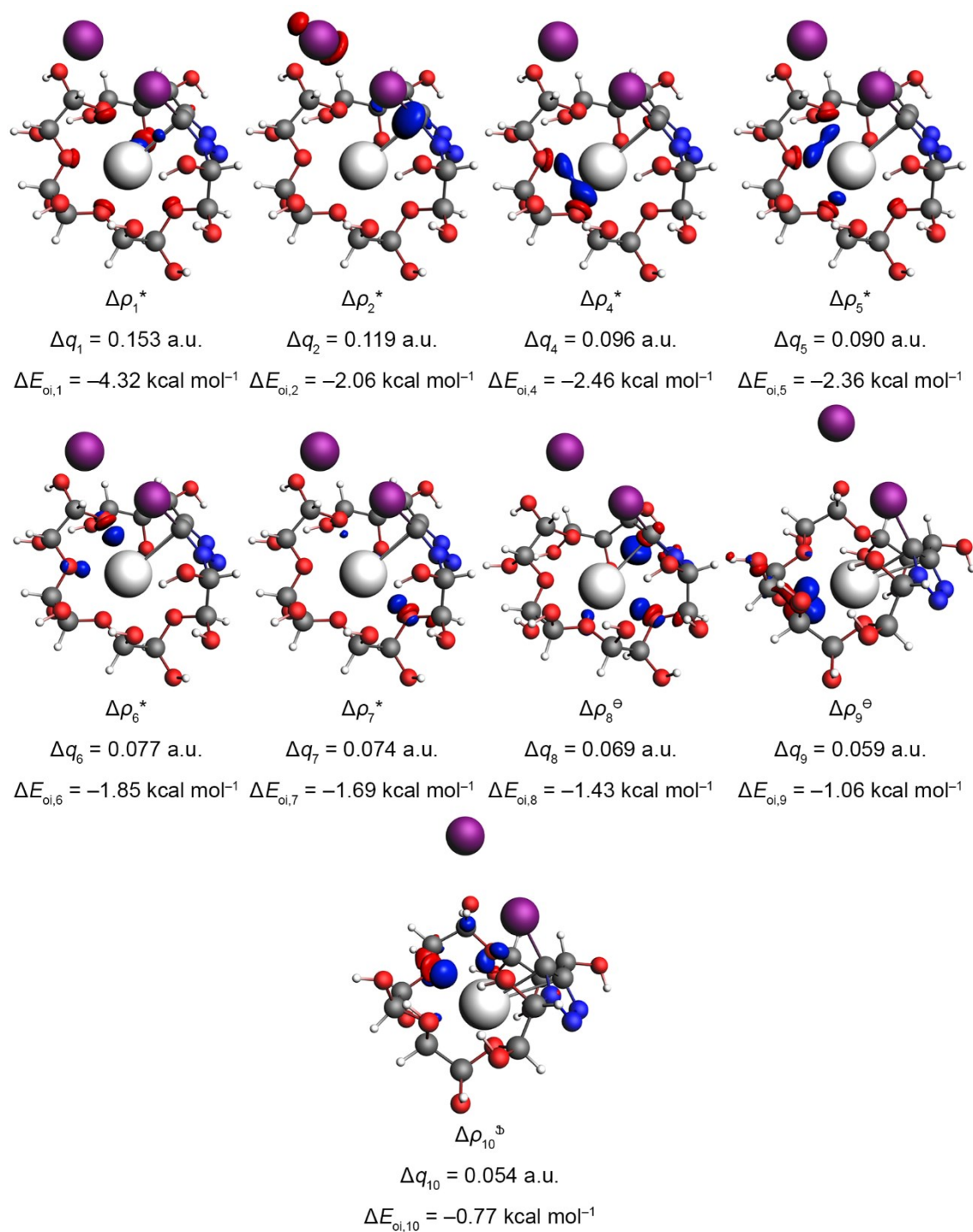


Figure S6. Selected density flow channels: $\Delta\rho_{1, 2}$ and 4–10 for $\text{Na}^+ \cdots 7\text{-I}^-$, with their respective energy, $\Delta E_{\text{oi},k}$, and charge transfer estimation, Δq_k . Red and blue regions indicate the electronic density outflow and inflow, respectively. The isovalues used to represent these surfaces are equal to: $*$ = 0.0010; Θ = 0.0005 and Φ = 0.0003 a.u.

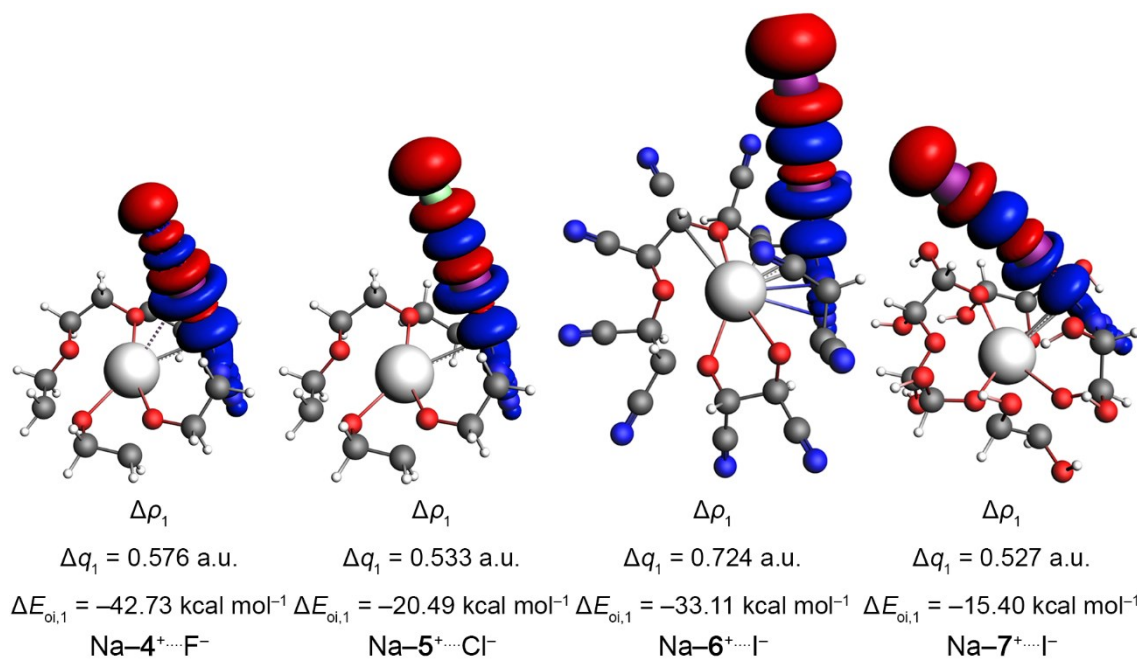


Figure S7. Selected density flow channels: $\Delta\rho_1$ for Na-4⁺...F⁻, Na-5⁺...Cl⁻, Na-6⁺...I⁻ and Na-7⁺...I⁻, with their respective energy, $\Delta E_{oi,k}$, and charge transfer estimation, Δq_k . Red and blue regions indicate the electronic density outflow and inflow, respectively. The isovalue used to represent these surfaces is equal to 0.0010 a.u.

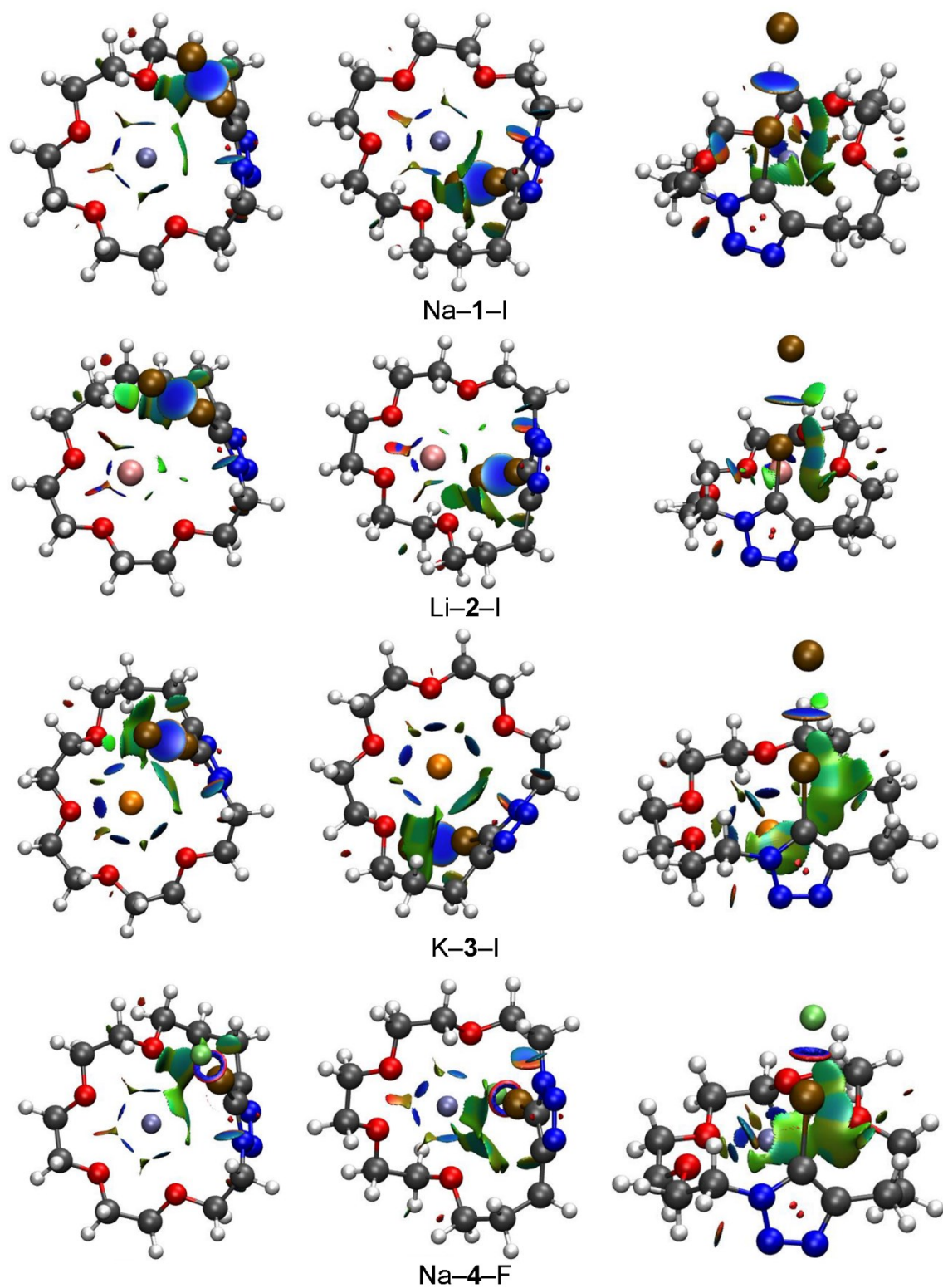


Figure S8. Different perspective (top, bottom and lateral) of NCI interactions in: Na-1-I, Li-2-I, K-3-I and Na-4-F. Red, blue and green surfaces represent repulsive, attractive and dispersion interactions, respectively.

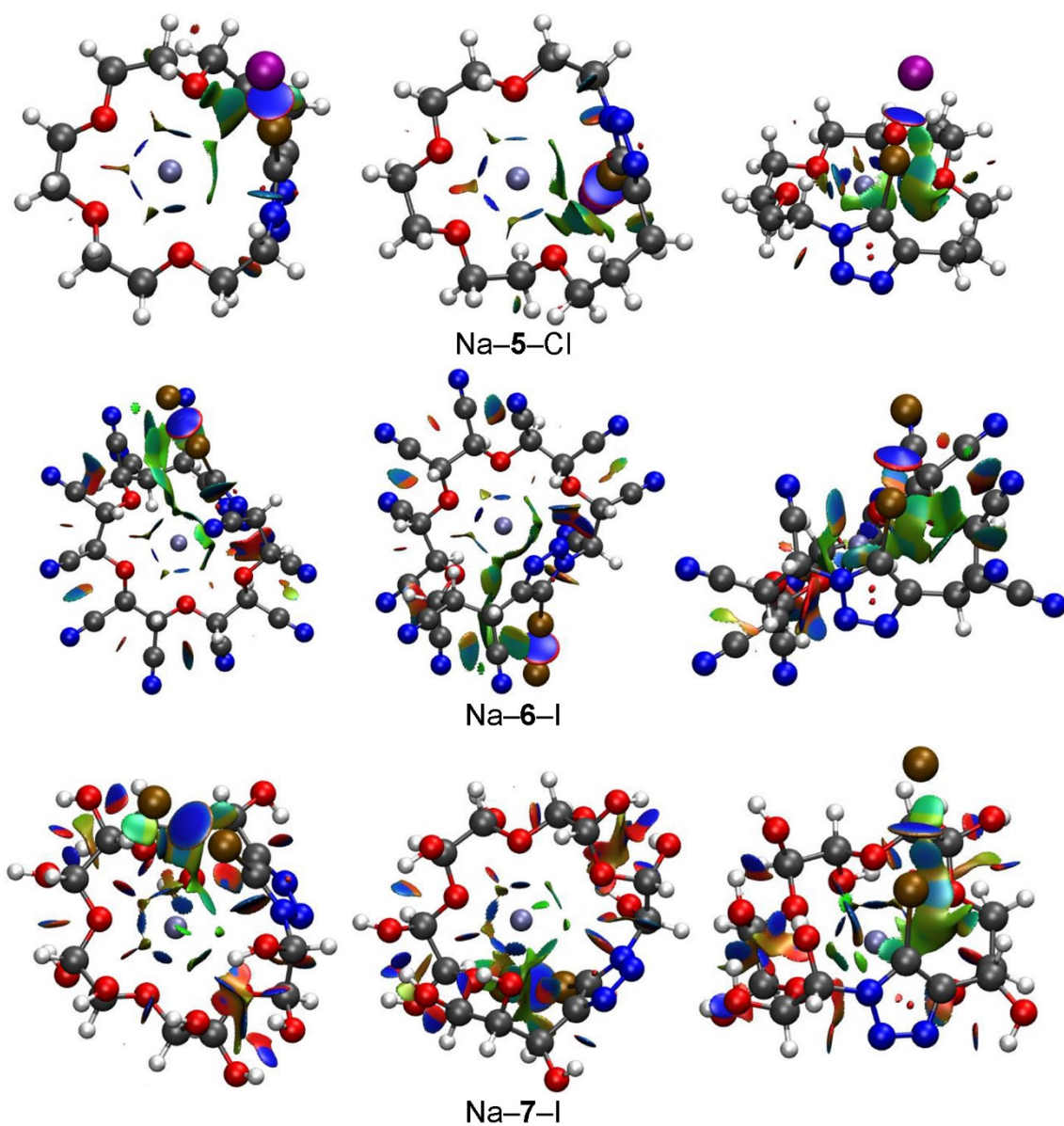


Figure S9. Different perspective (top, bottom and lateral) of NCI interactions in: Na-5-Cl, Na-6-I, and Na-7-I. Red, blue and green surfaces represent repulsive, attractive and dispersion interactions, respectively.