

**Supporting Information for**  
**The Effect of Ring Sizes and Alkali Metal Cations on Interaction**  
**Energy, Charge Transfer and Nonlinear Optical Properties of Crown**  
**Ether Derivatives**

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Table S1. The detailed O–M and O–O distances of compounds **1**, **2** and **3** and **N\*M** (N = 1, 2 and 3, M = Li<sup>+</sup>, Na<sup>+</sup> and K<sup>+</sup>).

	<b>1</b>	<b>1*Li</b>	<b>1*Na</b>	<b>1*K</b>
O3–M		1.909	2.340	2.752
O4–M		1.897	2.435	3.366
O1–M		1.907	2.303	2.722
O2–M		1.877	2.230	2.602
O1–O3	3.047	3.816	4.000	3.836
O2–O4	4.633	3.297	3.704	4.000
	<b>2</b>	<b>2*Li</b>	<b>2*Na</b>	<b>2*K</b>
O4–M		2.185	2.308	2.736
O1–M		2.224	2.298	2.680
O3–M		2.194	2.311	2.710
O2–M		2.215	2.296	2.677
O5–M		2.213	2.313	2.708
O2–O4	4.403	4.194	4.375	4.666
O1–O4	4.431	4.196	4.376	4.656
O2–O5	4.443	4.181	4.364	4.344
O3–O5	4.642	4.209	4.392	4.102
O1–O3	4.495	4.184	4.363	4.326
	<b>3</b>	<b>3*Li</b>	<b>3*Na</b>	<b>3*K</b>
O5–M		2.072	2.535	2.75
O6–M		2.145	2.571	2.725
O1–M		2.161	2.712	2.758
O2–M		2.111	2.746	2.782
O3–M		2.289	2.611	2.739
O4–M		2.125	2.683	2.755
O3–O6	5.055	3.516	5.123	5.451
O1–O4	5.852	3.460	5.393	5.492
O2–O5	6.101	4.172	5.272	5.444

Table S2. The topological properties and energy properties at the bond critical points (BCPs) of O–M.  
(All values are in unites of au).

	<b>1*Li</b>	<b>1*Na</b>	<b>1*K</b>
$\rho_b$ O1–M	0.0320	0.0217	0.0167
$\rho_b$ O2–M	0.0342	0.0260	0.0224
$\rho_b$ O3–M	0.0319	0.0207	0.0165
$\rho_b$ O4–M	0.0330	0.0166	
$\nabla^2\rho_b$ O1–M	0.2347	0.1352	0.0742
$\nabla^2\rho_b$ O2–M	0.2602	0.1725	0.1018
$\nabla^2\rho_b$ O3–M	0.2324	0.1228	0.0699
$\nabla^2\rho_b$ O4–M	0.2446	0.0947	
	<b>2*Li</b>	<b>2*Na</b>	<b>2*K</b>
$\rho_b$ O1–M	0.0137	0.0218	0.0184
$\rho_b$ O2–M	0.0134	0.0217	0.0183
$\rho_b$ O3–M	0.0144	0.0217	0.0182
$\rho_b$ O4–M	0.0154	0.0220	0.0166
$\rho_b$ O5–M	0.0151	0.0218	0.0181
$\nabla^2\rho_b$ O1–M	0.0843	0.1370	0.0833
$\nabla^2\rho_b$ O2–M	0.0821	0.1364	0.0827
$\nabla^2\rho_b$ O3–M	0.0860	0.1327	0.0793
$\nabla^2\rho_b$ O4–M	0.0932	0.1346	0.0728
$\nabla^2\rho_b$ O5–M	0.097	0.1332	0.0789
	<b>3*Li</b>	<b>3*Na</b>	<b>3*K</b>
$\rho_b$ O1–M	0.0162	0.0080	0.0157
$\rho_b$ O2–M	0.0175	0.0074	0.0149
$\rho_b$ O3–M	0.0178	0.0106	0.0173
$\rho_b$ O4–M		0.0090	0.0164
$\rho_b$ O5–M	0.0205	0.0121	0.0162
$\rho_b$ O6–M	0.0171	0.0117	0.0177
$\nabla^2\rho_b$ O1–M	0.1007	0.0428	0.0679
$\nabla^2\rho_b$ O2–M	0.1140	0.0395	0.0643
$\nabla^2\rho_b$ O3–M	0.1117	0.0558	0.0726
$\nabla^2\rho_b$ O4–M		0.0477	0.0693
$\nabla^2\rho_b$ O5–M	0.1324	0.0665	0.0693
$\nabla^2\rho_b$ O6–M	0.1062	0.0626	0.0748

## Optimized Structures

### Compound 1

6	0	0.109787	-1.264943	0.101350
6	0	0.986457	-0.185688	-0.150614
6	0	2.362583	-0.376590	-0.166330
6	0	2.902889	-1.669569	0.051246
6	0	2.044171	-2.731582	0.306067
6	0	0.663189	-2.533034	0.337442
6	0	-1.344265	-1.115767	0.131064
6	0	-2.051524	0.010729	-0.121023
1	0	0.584657	0.806280	-0.320204
1	0	2.475901	-3.710618	0.490002
1	0	0.005030	-3.373960	0.539561
1	0	-1.533872	0.930709	-0.383061
6	0	-5.803542	-0.027671	0.083942
6	0	-5.381684	1.264260	-0.276566
6	0	-6.298574	2.292030	-0.496581
6	0	-7.657450	2.001226	-0.347471
6	0	-8.082523	0.716727	0.011668
6	0	-7.153642	-0.311372	0.230671
6	0	-4.560965	-0.884797	0.241748
6	0	-3.489744	0.179166	-0.092744
1	0	-5.954446	3.283652	-0.774326
1	0	-8.394980	2.782336	-0.512269
1	0	-9.144285	0.513264	0.122113
1	0	-7.496480	-1.305598	0.509232
7	0	-3.982973	1.356794	-0.374630
6	0	-4.564388	-2.050826	-0.773677
1	0	-5.414559	-2.713842	-0.577137
1	0	-3.649261	-2.647612	-0.709839
1	0	-4.656213	-1.677570	-1.798636
6	0	-4.431337	-1.407846	1.690637
1	0	-5.278148	-2.061594	1.928991
1	0	-4.430513	-0.580517	2.407420
1	0	-3.510817	-1.982266	1.833645
6	0	5.000950	-1.649230	-1.114498
6	0	6.362845	-1.037712	-0.816186
6	0	2.920141	1.966826	-0.401600
6	0	4.208636	2.772317	-0.329600
6	0	6.092639	2.151377	1.071864
6	0	6.222753	0.642645	0.887859
1	0	5.362114	0.140754	1.342046
1	0	6.773431	2.657527	0.370365

1	0	5.142063	-2.625761	-1.601878		
1	0	6.973073	-1.131726	-1.724137		
1	0	2.370648	2.201310	-1.325674		
1	0	3.970157	3.828199	-0.526956		
8	0	6.323739	0.343705	-0.501623		
8	0	4.772608	2.665313	0.969262		
8	0	3.289681	0.593669	-0.376650		
8	0	4.261499	-1.856941	0.103951		
1	0	4.449341	-0.994304	-1.793333		
1	0	6.860235	-1.609624	-0.017941		
1	0	7.138105	0.300611	1.402050		
1	0	6.408838	2.404763	2.089760		
1	0	4.902415	2.419266	-1.099800		
1	0	2.282546	2.206697	0.459095		
1	0		-1.878810	-2.027971	0.381788	

Compound 2

6	0	-0.719568	-1.210650	-0.277629
6	0	0.124264	-0.121269	-0.600521
6	0	1.492798	-0.288856	-0.748754
6	0	2.070996	-1.578001	-0.576009
6	0	1.245528	-2.655036	-0.260064
6	0	-0.131454	-2.470465	-0.112187
6	0	-2.162913	-1.077252	-0.108629
6	0	-2.901741	0.050290	-0.246181
1	0	-0.304882	0.864671	-0.731434
1	0	1.669596	-3.643781	-0.125137
1	0	-0.756453	-3.324344	0.136592
1	0	-2.418848	0.986992	-0.515270
6	0	-6.616553	-0.051539	0.309315
6	0	-6.245301	1.260221	-0.035282
6	0	-7.191890	2.280881	-0.124640
6	0	-8.527103	1.962908	0.139748
6	0	-8.901234	0.658713	0.483731
6	0	-7.943004	-0.362242	0.570882
6	0	-5.354524	-0.894598	0.313944
6	0	-4.331349	0.198210	-0.076389
1	0	-6.887834	3.288305	-0.392289
1	0	-9.286031	2.738530	0.077670
1	0	-9.945208	0.434062	0.685380
1	0	-8.245635	-1.372384	0.838921
7	0	-4.863732	1.378929	-0.260805
6	0	-5.441576	-2.019791	-0.742459
1	0	-6.264183	-2.700636	-0.495422
1	0	-4.519421	-2.607304	-0.788682
1	0	-5.631592	-1.607123	-1.738394
6	0	-5.082767	-1.470163	1.722624
1	0	-5.891188	-2.151981	2.010818
1	0	-5.032531	-0.670720	2.468724
1	0	-4.141615	-2.027185	1.758569
6	0	7.171038	-1.002213	0.636177
6	0	7.152677	0.352623	1.321550
6	0	1.959931	2.054141	-0.904524
6	0	3.198938	2.925454	-0.985765
6	0	5.278382	3.271268	0.114392
6	0	6.191400	2.511156	1.059864
1	0	5.681359	2.373839	2.026508
1	0	5.704630	3.228068	-0.899745
1	0	7.886970	-1.670362	1.145008
1	0	8.188683	0.675444	1.528867

1	0	1.257758	2.338484	-1.702537		
1	0	2.885457	3.983532	-1.035296		
6	0	5.591002	-2.497481	-0.328053		
6	0	4.106142	-2.806519	-0.302884		
1	0	5.866479	-2.112887	-1.322555		
1	0	3.797558	-3.074681	0.716140		
8	0	6.495950	1.265611	0.469027		
8	0	3.416011	-1.641291	-0.736150		
8	0	3.997362	2.673964	0.148300		
8	0	2.372729	0.701951	-1.052242		
8	0	5.864426	-1.543146	0.671916		
1	0	3.893666	-3.655286	-0.970023		
1	0	6.151144	-3.434854	-0.160328		
1	0	7.511635	-0.868522	-0.401933		
1	0	6.627084	0.265501	2.285830		
1	0	7.108197	3.100225	1.241109		
1	0	5.226723	4.331864	0.415628		
1	0	3.749594	2.693029	-1.910976		
1	0	1.464631	2.196593	0.065053		
1		0	-2.664164	-2.005075	0.154500	

Compound 3

6	0	-1.491578	-1.310058	-0.408447
6	0	-0.624255	-0.254833	-0.777757
6	0	0.724710	-0.476388	-1.012520
6	0	1.263900	-1.784631	-0.856044
6	0	0.411849	-2.830467	-0.505904
6	0	-0.947474	-2.593642	-0.286139
6	0	-2.916189	-1.118912	-0.155532
6	0	-3.610739	0.042307	-0.227095
1	0	-1.021824	0.747062	-0.880110
1	0	0.798876	-3.836990	-0.397247
1	0	-1.591388	-3.424864	-0.010435
1	0	-3.101585	0.964325	-0.498671
6	0	-7.294706	0.083656	0.512041
6	0	-6.882882	1.388090	0.186487
6	0	-7.786721	2.450479	0.172098
6	0	-9.120621	2.181780	0.491952
6	0	-9.535096	0.884875	0.816844
6	0	-8.619671	-0.178092	0.828864
6	0	-6.072510	-0.812480	0.430789
6	0	-5.022004	0.246742	0.020856
1	0	-7.451642	3.451588	-0.081798
1	0	-9.846802	2.990508	0.488674
1	0	-10.577263	0.698923	1.062438
1	0	-8.953309	-1.182112	1.082783
7	0	-5.509895	1.454146	-0.103969
6	0	-6.259365	-1.900210	-0.651403
1	0	-7.098266	-2.552980	-0.384012
1	0	-5.366749	-2.523996	-0.758745
1	0	-6.478236	-1.449787	-1.624806
6	0	-5.759287	-1.441569	1.807596
1	0	-6.585039	-2.091886	2.118526
1	0	-5.632069	-0.667661	2.571250
1	0	-4.846370	-2.044174	1.779690
1	0	-3.442320	-2.030363	0.116306
6	0	1.235876	1.841801	-1.317127
6	0	2.423832	2.676657	-1.752019
6	0	6.684272	1.101024	2.290881
6	0	6.870609	2.486910	1.684817
6	0	5.837320	2.415914	-0.462663
6	0	4.710202	3.032680	-1.264955
1	0	4.884370	2.805870	-2.330779
1	0	6.798022	2.678432	-0.939851
1	0	0.387569	2.053379	-1.984656



1	0	2.723532	2.374925	-2.769672
1	0	5.695454	1.037513	2.771478
1	0	6.932593	3.208420	2.508531
6	0	3.228558	-3.135077	-0.749134
6	0	4.732425	-2.939533	-0.753914
1	0	2.917329	-3.480259	0.245319
1	0	5.202493	-3.937580	-0.702673
6	0	6.765643	-1.213235	1.781275
1	0	5.972900	-1.328184	2.536207
6	0	6.485865	-2.169940	0.636462
1	0	6.808280	-3.187724	0.918529
1	0	7.452568	0.954909	3.071928
1	0	7.826050	2.515070	1.134850
1	0	5.734416	1.325728	-0.473073
1	0	4.712390	4.128909	-1.147854
1	0	2.114387	3.736155	-1.795056
1	0	0.944259	2.092052	-0.288311
1	0	2.952364	-3.900842	-1.489578
1	0	5.052446	-2.464816	-1.694940
1	0	7.072106	-1.863651	-0.244420
1	0	7.727141	-1.471892	2.257348
8	0	5.804755	2.922546	0.865368
8	0	3.478881	2.478658	-0.842434
8	0	1.617295	0.473970	-1.396425
8	0	2.601950	-1.898343	-1.062644
8	0	5.097544	-2.155785	0.361978
8	0	6.807175	0.110689	1.284002

**1\*Li+**

6	0	-0.093571	-1.055586	0.090516
6	0	0.709344	0.083607	-0.133985
6	0	2.089118	-0.010907	-0.094157
6	0	2.721724	-1.243406	0.166454
6	0	1.950166	-2.381510	0.367931
6	0	0.560576	-2.281348	0.321305
6	0	-1.555795	-1.017628	0.072528
6	0	-2.316499	0.099630	0.010080
1	0	0.259337	1.041110	-0.373729
1	0	2.423511	-3.335846	0.576829
1	0	-0.034792	-3.175149	0.482741
1	0	-1.842736	1.078745	-0.023468
6	0	-6.064853	-0.100497	-0.034877
6	0	-5.678207	1.251274	-0.076126
6	0	-6.618277	2.281135	-0.125344
6	0	-7.969325	1.928500	-0.132833
6	0	-8.360438	0.583875	-0.092433
6	0	-7.408746	-0.444935	-0.042813
6	0	-4.800707	-0.938815	0.014417
6	0	-3.761348	0.200106	-0.010658
1	0	-6.297991	3.317835	-0.156253
1	0	-8.727936	2.704988	-0.170368
1	0	-9.417602	0.334008	-0.099450
1	0	-7.730205	-1.483341	-0.011608
7	0	-4.281898	1.397682	-0.061115
6	0	-4.692122	-1.853849	-1.227584
1	0	-5.520004	-2.570994	-1.234735
1	0	-3.756124	-2.422005	-1.232363
1	0	-4.742517	-1.270368	-2.152213
6	0	-4.735215	-1.763007	1.321399
1	0	-5.568829	-2.472680	1.355057
1	0	-4.807563	-1.114668	2.200214
1	0	-3.805116	-2.335945	1.394578
6	0	4.975763	-2.197233	-0.306102
6	0	6.393166	-1.652025	-0.128982
6	0	3.009015	2.189524	0.526762
6	0	4.350650	2.868313	0.265907
6	0	6.652875	2.012078	-0.132926
6	0	7.316338	0.637496	-0.047125
1	0	7.447764	0.357097	1.004136
1	0	6.563901	2.347118	-1.177154
1	0	4.884050	-3.156968	0.212671

1	0	7.113714	-2.307137	-0.630810
1	0	2.185937	2.891930	0.363409
1	0	4.503046	3.692762	0.972144
8	0	6.448882	-0.322485	-0.692133
8	0	5.348321	1.849265	0.444085
8	0	2.911943	1.081376	-0.412036
8	0	4.109875	-1.202098	0.282406
1	0	4.715054	-2.335006	-1.363494
1	0	6.636225	-1.602387	0.938711
1	0	8.294366	0.653323	-0.539908
1	0	7.244710	2.749452	0.422528
1	0	4.394671	3.264462	-0.758621
1	0	2.961354	1.799258	1.548631
1	0	-2.034832	-1.990344	0.130454
3	0	4.679315	0.379914	-0.552281

**1\*Na<sup>+</sup>**

6	0	-0.093571	-1.055586	0.090516
6	0	0.709344	0.083607	-0.133985
6	0	2.089118	-0.010907	-0.094157
6	0	2.721724	-1.243406	0.166454
6	0	1.950166	-2.381510	0.367931
6	0	0.560576	-2.281348	0.321305
6	0	-1.555795	-1.017628	0.072528
6	0	-2.316499	0.099630	0.010080
1	0	0.259337	1.041110	-0.373729
1	0	2.423511	-3.335846	0.576829
1	0	-0.034792	-3.175149	0.482741
1	0	-1.842736	1.078745	-0.023468
6	0	-6.064853	-0.100497	-0.034877
6	0	-5.678207	1.251274	-0.076126
6	0	-6.618277	2.281135	-0.125344
6	0	-7.969325	1.928500	-0.132833
6	0	-8.360438	0.583875	-0.092433
6	0	-7.408746	-0.444935	-0.042813
6	0	-4.800707	-0.938815	0.014417
6	0	-3.761348	0.200106	-0.010658
1	0	-6.297991	3.317835	-0.156253
1	0	-8.727936	2.704988	-0.170368
1	0	-9.417602	0.334008	-0.099450
1	0	-7.730205	-1.483341	-0.011608
7	0	-4.281898	1.397682	-0.061115
6	0	-4.692122	-1.853849	-1.227584
1	0	-5.520004	-2.570994	-1.234735
1	0	-3.756124	-2.422005	-1.232363
1	0	-4.742517	-1.270368	-2.152213
6	0	-4.735215	-1.763007	1.321399
1	0	-5.568829	-2.472680	1.355057
1	0	-4.807563	-1.114668	2.200214
1	0	-3.805116	-2.335945	1.394578
6	0	4.975763	-2.197233	-0.306102
6	0	6.393166	-1.652025	-0.128982
6	0	3.009015	2.189524	0.526762
6	0	4.350650	2.868313	0.265907
6	0	6.652875	2.012078	-0.132926
6	0	7.316338	0.637496	-0.047125
1	0	7.447764	0.357097	1.004136
1	0	6.563901	2.347118	-1.177154
1	0	4.884050	-3.156968	0.212671
1	0	7.113714	-2.307137	-0.630810

1	0	2.185937	2.891930	0.363409
1	0	4.503046	3.692762	0.972144
8	0	6.448882	-0.322485	-0.692133
8	0	5.348321	1.849265	0.444085
8	0	2.911943	1.081376	-0.412036
8	0	4.109875	-1.202098	0.282406
1	0	4.715054	-2.335006	-1.363494
1	0	6.636225	-1.602387	0.938711
1	0	8.294366	0.653323	-0.539908
1	0	7.244710	2.749452	0.422528
1	0	4.394671	3.264462	-0.758621
1	0	2.961354	1.799258	1.548631
1	0	-2.034832	-1.990344	0.130454
3	0	4.679315	0.379914	-0.552281

1*K <sup>+</sup>				
6	0	-0.093571	-1.055586	0.090516
6	0	0.709344	0.083607	-0.133985
6	0	2.089118	-0.010907	-0.094157
6	0	2.721724	-1.243406	0.166454
6	0	1.950166	-2.381510	0.367931
6	0	0.560576	-2.281348	0.321305
6	0	-1.555795	-1.017628	0.072528
6	0	-2.316499	0.099630	0.010080
1	0	0.259337	1.041110	-0.373729
1	0	2.423511	-3.335846	0.576829
1	0	-0.034792	-3.175149	0.482741
1	0	-1.842736	1.078745	-0.023468
6	0	-6.064853	-0.100497	-0.034877
6	0	-5.678207	1.251274	-0.076126
6	0	-6.618277	2.281135	-0.125344
6	0	-7.969325	1.928500	-0.132833
6	0	-8.360438	0.583875	-0.092433
6	0	-7.408746	-0.444935	-0.042813
6	0	-4.800707	-0.938815	0.014417
6	0	-3.761348	0.200106	-0.010658
1	0	-6.297991	3.317835	-0.156253
1	0	-8.727936	2.704988	-0.170368
1	0	-9.417602	0.334008	-0.099450
1	0	-7.730205	-1.483341	-0.011608
7	0	-4.281898	1.397682	-0.061115
6	0	-4.692122	-1.853849	-1.227584
1	0	-5.520004	-2.570994	-1.234735
1	0	-3.756124	-2.422005	-1.232363
1	0	-4.742517	-1.270368	-2.152213
6	0	-4.735215	-1.763007	1.321399
1	0	-5.568829	-2.472680	1.355057
1	0	-4.807563	-1.114668	2.200214
1	0	-3.805116	-2.335945	1.394578
6	0	4.975763	-2.197233	-0.306102
6	0	6.393166	-1.652025	-0.128982
6	0	3.009015	2.189524	0.526762
6	0	4.350650	2.868313	0.265907
6	0	6.652875	2.012078	-0.132926
6	0	7.316338	0.637496	-0.047125
1	0	7.447764	0.357097	1.004136
1	0	6.563901	2.347118	-1.177154
1	0	4.884050	-3.156968	0.212671
1	0	7.113714	-2.307137	-0.630810

1	0	2.185937	2.891930	0.363409
1	0	4.503046	3.692762	0.972144
8	0	6.448882	-0.322485	-0.692133
8	0	5.348321	1.849265	0.444085
8	0	2.911943	1.081376	-0.412036
8	0	4.109875	-1.202098	0.282406
1	0	4.715054	-2.335006	-1.363494
1	0	6.636225	-1.602387	0.938711
1	0	8.294366	0.653323	-0.539908
1	0	7.244710	2.749452	0.422528
1	0	4.394671	3.264462	-0.758621
1	0	2.961354	1.799258	1.548631
1	0	-2.034832	-1.990344	0.130454
3	0	4.679315	0.379914	-0.552281

**2\*Li<sup>+</sup>**

6	0	-0.816684	-1.250773	-0.146537
6	0	0.032971	-0.132701	-0.314987
6	0	1.403143	-0.300682	-0.410577
6	0	1.977229	-1.582325	-0.335678
6	0	1.159630	-2.691547	-0.163987
6	0	-0.223794	-2.519136	-0.072096
6	0	-2.271593	-1.134420	-0.041608
6	0	-2.991500	0.006693	-0.138437
1	0	-0.396749	0.859665	-0.361694
1	0	1.577627	-3.689271	-0.096820
1	0	-0.852860	-3.394052	0.061826
1	0	-2.488893	0.955540	-0.315719
6	0	-6.732580	-0.026095	0.189052
6	0	-6.305172	1.294619	-0.036181
6	0	-7.210063	2.353706	-0.109249
6	0	-8.566892	2.063112	0.049527
6	0	-8.998490	0.749700	0.274402
6	0	-8.081703	-0.309134	0.346188
6	0	-5.499086	-0.910292	0.208035
6	0	-4.427694	0.171875	-0.039076
1	0	-6.859527	3.366046	-0.284488
1	0	-9.298255	2.864691	-0.002027
1	0	-10.059139	0.547971	0.394736
1	0	-8.433050	-1.323338	0.521167
7	0	-4.909143	1.379598	-0.168833
6	0	-5.548878	-1.954338	-0.931556
1	0	-6.400792	-2.626856	-0.783697
1	0	-4.641020	-2.565444	-0.962716
1	0	-5.667127	-1.468584	-1.905221
6	0	-5.328995	-1.594158	1.584448
1	0	-6.174104	-2.264683	1.774680
1	0	-5.297390	-0.853870	2.390089
1	0	-4.411235	-2.189263	1.631210
6	0	7.210838	-1.018925	0.283481
6	0	7.343170	0.337249	0.938698
6	0	1.863285	2.068873	-0.449273
6	0	3.059310	2.950117	-0.733110
6	0	5.325791	3.250714	-0.035469
6	0	6.383039	2.528498	0.768903
1	0	6.131822	2.532701	1.839236
1	0	5.625452	3.321047	-1.090923
1	0	7.826238	-1.763239	0.805940
1	0	8.365477	0.720675	0.821860



1	0	1.069177	2.280401	-1.173938
1	0	2.819038	3.993684	-0.490143
6	0	5.503603	-2.562326	-0.356483
6	0	4.030838	-2.824833	-0.134793
1	0	5.720164	-2.427427	-1.426267
1	0	3.825556	-3.103323	0.906170
8	0	6.404429	1.187361	0.280867
8	0	3.355816	-1.601182	-0.441878
8	0	4.132724	2.474079	0.077560
8	0	2.323399	0.719500	-0.576142
8	0	5.827966	-1.368159	0.352635
3	0	4.432273	0.303491	-0.042119
1	0	3.695729	-3.631485	-0.796548
1	0	6.092982	-3.411106	0.015475
1	0	7.530194	-0.970541	-0.767404
1	0	7.107501	0.279686	2.011030
1	0	7.361525	3.008324	0.634072
1	0	5.167806	4.264656	0.355121
1	0	3.344249	2.893617	-1.793808
1	0	1.478564	2.229259	0.565228
1	0	-2.784783	-2.076757	0.125620

**2\*Na<sup>+</sup>**

6	0	-0.982294	-1.278835	-0.183617
6	0	-0.130457	-0.169561	-0.385020
6	0	1.240636	-0.332446	-0.492257
6	0	1.816068	-1.620431	-0.400583
6	0	0.990048	-2.720189	-0.200926
6	0	-0.390876	-2.546896	-0.092833
6	0	-2.435257	-1.154729	-0.061895
6	0	-3.151198	-0.012433	-0.173487
1	0	-0.557584	0.823123	-0.451284
1	0	1.408542	-3.717519	-0.125949
1	0	-1.018720	-3.418776	0.064851
1	0	-2.646573	0.929574	-0.379077
6	0	-6.886693	-0.015256	0.213109
6	0	-6.455403	1.297114	-0.050362
6	0	-7.355115	2.359815	-0.134335
6	0	-8.710862	2.081568	0.053017
6	0	-9.146342	0.776570	0.316188
6	0	-8.234759	-0.285984	0.398564
6	0	-5.658138	-0.906376	0.233294
6	0	-4.584780	0.163054	-0.056607
1	0	-7.001486	3.365441	-0.339456
1	0	-9.438290	2.886192	-0.006088
1	0	-10.206061	0.584341	0.458281
1	0	-8.589292	-1.293478	0.603278
7	0	-5.061279	1.370370	-0.207001
6	0	-5.733050	-1.977267	-0.879703
1	0	-6.587096	-2.639548	-0.701485
1	0	-4.830083	-2.595613	-0.910500
1	0	-5.863813	-1.514470	-1.862882
6	0	-5.469112	-1.558173	1.622769
1	0	-6.313466	-2.220834	1.841780
1	0	-5.422432	-0.799295	2.410179
1	0	-4.552770	-2.155508	1.669270
6	0	7.103437	-1.049156	0.300894
6	0	7.262046	0.334056	0.908971
6	0	1.701838	2.056187	-0.437848
6	0	2.891317	2.972780	-0.668428
6	0	5.189404	3.272247	-0.004294
6	0	6.282427	2.539801	0.755263
1	0	6.034111	2.485846	1.825385
1	0	5.439657	3.318794	-1.074186
1	0	7.778261	-1.755088	0.803460
1	0	8.305330	0.662825	0.808596

1	0	0.899150	2.343361	-1.126756
1	0	2.595922	4.005986	-0.440059
6	0	5.369432	-2.627513	-0.258954
6	0	3.879462	-2.862432	-0.076878
1	0	5.605878	-2.496465	-1.325403
1	0	3.632574	-3.051938	0.975298
8	0	6.383592	1.220893	0.211582
8	0	3.195272	-1.683676	-0.524571
8	0	3.964838	2.554195	0.177177
8	0	2.132665	0.710951	-0.691476
8	0	5.740176	-1.452921	0.465295
11	0	4.293513	0.277215	-0.046217
1	0	3.584932	-3.732482	-0.675168
1	0	5.918328	-3.503764	0.112488
1	0	7.358258	-1.022712	-0.768599
1	0	7.003393	0.313834	1.977808
1	0	7.232926	3.079080	0.644281
1	0	5.095826	4.297857	0.377330
1	0	3.208538	2.927278	-1.720952
1	0	1.333529	2.134373	0.592563
1	0	-2.950174	-2.090999	0.132078

**2\*K<sup>+</sup>**

6	0	-1.154772	-1.321372	-0.204718
6	0	-0.294959	-0.232302	-0.455065
6	0	1.080798	-0.396648	-0.546021
6	0	1.649272	-1.681690	-0.398327
6	0	0.807438	-2.767599	-0.166419
6	0	-0.570729	-2.589601	-0.067167
6	0	-2.606874	-1.182030	-0.084535
6	0	-3.304303	-0.024240	-0.138106
1	0	-0.717965	0.756489	-0.580586
1	0	1.221898	-3.763806	-0.058619
1	0	-1.202435	-3.452627	0.121894
1	0	-2.782222	0.919481	-0.283157
6	0	-7.043006	0.015563	0.217930
6	0	-6.586434	1.334042	0.042800
6	0	-7.466785	2.415836	0.020801
6	0	-8.828834	2.150553	0.179530
6	0	-9.289446	0.839426	0.354477
6	0	-8.397167	-0.242356	0.375163
6	0	-5.830235	-0.896728	0.191515
6	0	-4.735541	0.169360	-0.019997
1	0	-7.093871	3.426149	-0.115789
1	0	-9.541487	2.970367	0.167299
1	0	-10.353575	0.657551	0.475826
1	0	-8.770800	-1.254475	0.512091
7	0	-5.189781	1.392095	-0.097938
6	0	-5.909976	-1.891728	-0.989413
1	0	-6.775587	-2.551185	-0.863746
1	0	-5.015435	-2.519846	-1.051155
1	0	-6.023074	-1.363790	-1.941521
6	0	-5.668256	-1.640463	1.537506
1	0	-6.530190	-2.294699	1.707937
1	0	-5.609678	-0.934791	2.372171
1	0	-4.767294	-2.262189	1.551644
6	0	6.889642	-1.038015	0.734265
6	0	7.037989	0.366274	1.293526
6	0	1.563209	1.953408	-0.307404
6	0	2.724110	2.914551	-0.493286
6	0	5.008222	3.238389	0.192905
6	0	6.082204	2.547832	1.015256
1	0	6.975186	3.186826	1.069186
1	0	5.357022	3.412258	-0.839277
1	0	7.354627	-1.112928	-0.263357
1	0	8.104511	0.609704	1.403050

1	0	0.701906	2.346338	-0.860480
1	0	2.430135	3.897161	-0.096364
6	0	5.166545	-2.634491	0.205860
6	0	3.660544	-2.810503	0.290154
1	0	5.516816	-2.784789	-0.830091
1	0	3.319768	-2.710851	1.327169
8	0	6.393562	1.289658	0.415703
8	0	3.026163	-1.803023	-0.514744
8	0	3.855333	2.401351	0.197319
8	0	1.943951	0.659267	-0.802360
8	0	5.496708	-1.329212	0.660812
19	0	4.540999	0.258712	-1.313076
1	0	3.410743	-3.814640	-0.072665
1	0	5.643799	-3.403698	0.830476
1	0	7.404414	-1.748008	1.397379
1	0	6.567748	0.407314	2.285360
1	0	5.705266	2.389789	2.034832
1	0	4.784162	4.217896	0.639166
1	0	2.951284	3.045574	-1.565642
1	0	1.297952	1.870552	0.752875
1	0	-3.135821	-2.118462	0.066871

**3\*Li<sup>+</sup>**

6	0	-1.195355	-1.080636	-0.431677
6	0	-0.351416	0.043898	-0.306633
6	0	1.019977	-0.081855	-0.443659
6	0	1.606133	-1.334279	-0.693824
6	0	0.796096	-2.460695	-0.807129
6	0	-0.587171	-2.323399	-0.679910
6	0	-2.651136	-1.009683	-0.299827
6	0	-3.379122	0.110911	-0.090383
1	0	-0.760336	1.023609	-0.082527
1	0	1.222628	-3.438734	-1.000952
1	0	-1.210302	-3.208088	-0.774334
1	0	-2.883002	1.075877	-0.007644
6	0	-7.118129	-0.047665	0.222010
6	0	-6.705117	1.289778	0.356297
6	0	-7.620980	2.319818	0.571141
6	0	-8.974017	1.982374	0.650223
6	0	-9.391192	0.651942	0.517388
6	0	-8.463440	-0.377307	0.301451
6	0	-5.876205	-0.891845	0.001091
6	0	-4.816515	0.229004	0.050795
1	0	-7.281292	3.345870	0.672257
1	0	-9.713499	2.760479	0.816933
1	0	-10.449065	0.413535	0.582555
1	0	-8.803774	-1.405311	0.200486
7	0	-5.310678	1.422188	0.247995
6	0	-5.921995	-1.592089	-1.376937
1	0	-6.767201	-2.288017	-1.412567
1	0	-5.008846	-2.163559	-1.572857
1	0	-6.049529	-0.864300	-2.184437
6	0	-5.694892	-1.919624	1.142046
1	0	-6.536887	-2.620321	1.148272
1	0	-5.660748	-1.423510	2.117063
1	0	-4.775109	-2.501437	1.022270
1	0	-3.158046	-1.966278	-0.385464
6	0	1.856569	2.010902	-1.310447
6	0	2.911429	1.690369	-2.363572
6	0	4.755313	0.903370	2.816338
6	0	5.757216	1.637162	1.931619
6	0	5.876008	2.428493	-0.347603
6	0	4.928922	2.702971	-1.499455
1	0	5.487105	2.998960	-2.396819
1	0	6.404902	3.348614	-0.065618
1	0	0.861763	2.071456	-1.763290

1	0	2.676784	0.748118	-2.865325
1	0	3.957425	1.589621	3.113955
1	0	6.105187	2.551030	2.433422
6	0	3.697285	-2.549159	-0.917679
6	0	5.170173	-2.166536	-1.007099
1	0	3.482390	-3.181601	-0.046747
1	0	5.796476	-3.066968	-0.964688
6	0	4.626527	-1.480716	2.254827
1	0	3.786220	-2.142279	2.028124
6	0	5.805273	-1.749923	1.314636
1	0	6.017989	-2.826394	1.277480
1	0	5.244094	0.523411	3.721633
1	0	6.633881	1.016047	1.702412
1	0	6.614759	1.660965	-0.618076
1	0	4.247443	3.517441	-1.224964
1	0	2.957513	2.482577	-3.121978
1	0	2.065985	2.957032	-0.804532
1	0	3.398890	-3.093654	-1.822435
1	0	5.360426	-1.655495	-1.954541
1	0	6.710147	-1.248903	1.672442
1	0	4.925546	-1.661109	3.296099
8	0	5.062885	1.955998	0.727538
8	0	4.193640	1.497529	-1.748607
8	0	1.876031	1.003709	-0.273101
8	0	2.982119	-1.317702	-0.807348
8	0	5.550926	-1.231534	0.003332
8	0	4.105448	-0.158360	2.103538
3	0	3.915001	0.368469	0.053808

**3\*Na<sup>+</sup>**

6	0	-1.599748	-1.395251	-0.209946
6	0	-0.736457	-0.330125	-0.556118
6	0	0.623607	-0.540965	-0.712099
6	0	1.174499	-1.825409	-0.524254
6	0	0.338306	-2.883199	-0.185473
6	0	-1.033641	-2.664440	-0.033524
6	0	-3.041681	-1.222213	-0.029788
6	0	-3.726161	-0.058999	-0.120926
1	0	-1.148618	0.659958	-0.702559
1	0	0.735506	-3.880882	-0.039132
1	0	-1.672563	-3.502091	0.230559
1	0	-3.200376	0.866602	-0.346821
6	0	-7.443773	0.047731	0.405353
6	0	-6.984743	1.347455	0.127579
6	0	-7.856630	2.435095	0.078647
6	0	-9.212200	2.195259	0.315701
6	0	-9.675073	0.902859	0.592865
6	0	-8.791257	-0.185022	0.640070
6	0	-6.241320	-0.878195	0.379571
6	0	-5.148253	0.160634	0.051135
1	0	-7.482386	3.430886	-0.137824
1	0	-9.917804	3.020724	0.284764
1	0	-10.733904	0.740384	0.773726
1	0	-9.166174	-1.182741	0.856482
7	0	-5.595486	1.381226	-0.081070
6	0	-6.386978	-1.943852	-0.731187
1	0	-7.252422	-2.582251	-0.522831
1	0	-5.503010	-2.586419	-0.795602
1	0	-6.540437	-1.474866	-1.708168
6	0	-6.022242	-1.538537	1.760476
1	0	-6.879459	-2.173321	2.010294
1	0	-5.921076	-0.783051	2.546035
1	0	-5.125253	-2.165994	1.772526
1	0	-3.576545	-2.138542	0.202627
6	0	1.038883	1.714552	-1.423470
6	0	2.218102	2.526701	-1.907336
6	0	6.608575	0.926876	2.127972
6	0	6.449690	2.327558	1.576135
6	0	4.932055	3.652440	0.296744
6	0	4.223232	3.502177	-1.033306
1	0	4.919676	3.142724	-1.806734
1	0	4.282628	4.148830	1.030309
1	0	0.295196	1.619035	-2.224313



1	0	2.662552	2.075272	-2.807248
1	0	5.832030	0.707642	2.877619
1	0	6.368974	3.042868	2.406873
6	0	3.136216	-3.198054	-0.634624
6	0	4.604701	-3.027714	-0.952201
1	0	3.015270	-3.613866	0.374028
1	0	5.105279	-4.000831	-0.853354
6	0	6.902733	-1.303443	1.339594
1	0	6.374750	-1.670757	2.232488
6	0	6.552947	-2.164861	0.147853
1	0	6.862466	-3.202021	0.338334
1	0	7.589795	0.837337	2.615493
1	0	7.322350	2.598718	0.965008
1	0	5.832214	4.265327	0.155257
1	0	3.826819	4.476660	-1.351936
1	0	1.879295	3.541245	-2.159960
1	0	0.572297	2.202483	-0.558224
1	0	2.670760	-3.877767	-1.359775
1	0	4.746776	-2.668907	-1.982208
1	0	7.070061	-1.806722	-0.754556
1	0	7.984587	-1.343209	1.532719
8	0	5.277459	2.350274	0.767085
8	0	3.168521	2.565001	-0.847752
8	0	1.540035	0.431300	-1.052145
8	0	2.537393	-1.906260	-0.705379
8	0	5.139504	-2.090722	-0.021659
8	0	6.495796	0.024191	1.034582
11	0	4.059013	0.285851	-0.057901

**3\*K+**

6	0	-1.693169	-1.451324	-0.262021
6	0	-0.827087	-0.395857	-0.624590
6	0	0.532498	-0.603525	-0.802790
6	0	1.085063	-1.892286	-0.604370
6	0	0.238022	-2.940658	-0.255623
6	0	-1.130864	-2.721706	-0.090656
6	0	-3.130947	-1.267731	-0.060914
6	0	-3.807532	-0.098923	-0.137717
1	0	-1.239334	0.594543	-0.765198
1	0	0.629862	-3.939898	-0.109016
1	0	-1.767779	-3.558018	0.182341
1	0	-3.277724	0.823554	-0.367272
6	0	-7.516865	0.034800	0.437106
6	0	-7.050576	1.332767	0.163201
6	0	-7.913981	2.427852	0.132901
6	0	-9.268485	2.197280	0.384688
6	0	-9.738554	0.906629	0.657954
6	0	-8.863265	-0.188746	0.686462
6	0	-6.322615	-0.900786	0.390049
6	0	-5.225240	0.131302	0.055171
1	0	-7.534313	3.422141	-0.081006
1	0	-9.967641	3.028612	0.368331
1	0	-10.796426	0.751432	0.850395
1	0	-9.243737	-1.184967	0.900007
7	0	-5.663791	1.356534	-0.062669
6	0	-6.490227	-1.957725	-0.725945
1	0	-7.357743	-2.591098	-0.511003
1	0	-5.611900	-2.606290	-0.805531
1	0	-6.652281	-1.481091	-1.697809
6	0	-6.092233	-1.572393	1.763697
1	0	-6.952271	-2.200584	2.020277
1	0	-5.973662	-0.823281	2.552924
1	0	-5.201405	-2.208652	1.759945
1	0	-3.669423	-2.180762	0.176061
6	0	0.905992	1.698143	-1.429250
6	0	2.008751	2.527778	-2.072658
6	0	6.670137	1.143772	1.923254
6	0	6.354207	2.481210	1.283739
6	0	4.599995	3.740187	0.283218
6	0	3.188891	3.611092	-0.257390
1	0	2.870866	4.583252	-0.660508
1	0	4.635295	4.556787	1.019467
1	0	0.063878	1.646867	-2.130666

1	0	2.313386	2.056525	-3.012159
1	0	6.022988	0.976396	2.797817
1	0	6.560074	3.279764	2.011868
6	0	3.036762	-3.286759	-0.475231
6	0	4.540464	-3.189724	-0.638561
1	0	2.793689	-3.575791	0.554899
1	0	4.971203	-4.185716	-0.459166
6	0	6.852242	-1.183838	1.441339
1	0	6.342511	-1.402938	2.391530
6	0	6.467584	-2.222869	0.406473
1	0	6.846113	-3.206043	0.721670
1	0	7.714591	1.156969	2.267940
1	0	7.000435	2.640863	0.407417
1	0	5.286552	3.985840	-0.540393
1	0	2.498395	3.332214	0.552336
1	0	1.613975	3.527430	-2.303029
1	0	0.545739	2.146473	-0.493358
1	0	2.650432	-4.052643	-1.159839
1	0	4.802288	-2.887817	-1.665348
1	0	6.921149	-1.976745	-0.566380
1	0	7.937673	-1.225548	1.614201
8	0	4.984142	2.507806	0.889527
8	0	3.197353	2.626213	-1.290612
8	0	1.422684	0.388461	-1.171598
8	0	2.450883	-2.015204	-0.772848
8	0	5.045392	-2.248488	0.302656
8	0	6.474631	0.105945	0.964961
19	0	4.042979	0.221940	-0.325735