Electronic supplementary information

(35 pages including this page)

Title: Structural, energetic, spectroscopic and QTAIM analyses of cation-π interactions involving mono- and bi-cyclic ring fused benzene systems

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Table S6: Atomic Contributions to the Total Energy, E(Ω), of phenanthrene and triphenylene and their corresponding linear counterparts anthracene and naphthacene (in hartree) calculated with the Quantum Theory of Atoms in Molecules (QTAIM) at the B3LYP/6-311+G(2d,2p) level. (See Scheme 2 for atom numbering)

Table S7: Atomic energy (in hartrees), E(Ω) obtained with atomic integration of atomic basins by QTAIM at the B3LYP/6-311+G(2d,2p) level. The table lists the sum of atomic energy of all carbon atoms, $\sum E(\Omega_C)$; sum of atomic energy of all hydrogen atoms, $\sum E(\Omega_H)$; average energy of all hydrogen atoms, $\overline{E}_H$; and average energy of hydrogen atoms involved in hydrogen-hydrogen interaction, $\overline{E}_{H\cdots H}$; all these values are reported in hartrees. The following entities $\Delta E(\Omega_C)$, $\Delta E(\Omega_H)$, $[\Delta E(\Omega_H)+\Delta E(\Omega_C)]$, $\Delta \overline{E}_H$, $(\overline{E}_{H\cdots H} - \overline{E}_H)$ are reported in kcal/mol. (See Table S6 for individual atomic contributions to total energies of systems).

Table S8: Selected vibrational frequencies (ν_{C-H}, in cm^{-1}) corresponding to C–H bonds of bridge CH_2 unit (that is not on the side of metal ion binding) of bicyclo[2.1.1]hexenyl moiety of ligands (**5-7**) and their complexes obtained at the B3LYP/6-311+G(2d,2p) level. Intensities (km/mol) are given in parentheses.

Table S1: B3LYP/6-311+G(2d,2p) level optimized Cartesian coordinates of all the ligands and their complexes with the point group (PG).

1			PG: D_{6h}
C	0.000000	1.391490	0.000000
C	1.205066	0.695745	0.000000
C	1.205066	-0.695745	0.000000
C	0.000000	-1.391490	0.000000
C	-1.205066	-0.695745	0.000000
C	-1.205066	0.695745	0.000000
H	0.000000	2.472996	0.000000
H	2.141677	1.236498	0.000000
H	2.141677	-1.236498	0.000000
H	0.000000	-2.472996	0.000000
H	-2.141677	-1.236498	0.000000
H	-2.141677	1.236498	0.000000

1-Li$^+$			PG: C_{6v}
Li	0.000000	0.000000	1.718551
C	0.000000	1.399667	-0.122087
C	1.212147	0.699834	-0.122087
C	1.212147	-0.699834	-0.122087
C	0.000000	-1.399667	-0.122087
C	-1.212147	-0.699834	-0.122087
C	-1.212147	0.699834	-0.122087
H	0.000000	2.480699	-0.126751
H	2.148348	1.240349	-0.126751
H	2.148348	-1.240349	-0.126751
H	0.000000	-2.480699	-0.126751
H	-2.148348	-1.240349	-0.126751
H	-2.148348	1.240349	-0.126751

1-Na$^+$			PG: C_{6v}
Na	0.000000	0.000000	1.899069
C	0.000000	1.398028	-0.493365
C	1.210728	0.699014	-0.493365
C	1.210728	-0.699014	-0.493365
C	0.000000	-1.398028	-0.493365
C	-1.210728	-0.699014	-0.493365
C	-1.210728	0.699014	-0.493365
H	0.000000	2.479083	-0.521438
H	2.146949	1.239542	-0.521438
H	2.146949	-1.239542	-0.521438
H	0.000000	-2.479083	-0.521438
H	-2.146949	-1.239542	-0.521438
H	-2.146949	1.239542	-0.521438

1-K$^+$			PG: C_{6v}
K	0.000000	0.000000	1.986177
C	0.000000	1.396085	-0.893469
C	1.209045	0.698042	-0.893469
C	1.209045	-0.698042	-0.893469
C	0.000000	-1.396085	-0.893469
C	-1.209045	-0.698042	-0.893469
C	-1.209045	0.698042	-0.893469
H	0.000000	2.476907	-0.928743
H	2.145064	1.238454	-0.928743
H	2.145064	-1.238454	-0.928743
H	0.000000	-2.476907	-0.928743
H	-2.145064	-1.238454	-0.928743
H	-2.145064	1.238454	-0.928743

2			PG: D_{2h}
C	0.000000	1.241619	1.398264
C	0.000000	2.425848	0.706433
C	0.000000	2.425848	-0.706433
C	0.000000	1.241619	-1.398264
C	0.000000	-1.241619	-1.398264
C	0.000000	-2.425848	-0.706433
C	0.000000	-2.425848	0.706433
C	0.000000	-1.241619	1.398264
C	0.000000	0.000000	0.714465
C	0.000000	0.000000	-0.714465
H	0.000000	1.240740	2.480691
H	0.000000	3.366039	1.240859
H	0.000000	3.366039	-1.240859
H	0.000000	1.240740	-2.480691
H	0.000000	-1.240740	-2.480691
H	0.000000	-3.366039	-1.240859
H	0.000000	-3.366039	1.240859
H	0.000000	-1.240740	2.480691

2-Li^+			PG: Cs
Li	-1.708179	-1.276614	0.000000
C	0.108419	-1.186491	1.403292
C	0.152177	-2.379785	0.709525
C	0.152177	-2.379785	-0.709525
C	0.108419	-1.186491	-1.403292
C	0.032185	1.304455	-1.407357
C	0.008752	2.481532	-0.708023
C	0.008752	2.481532	0.708023
C	0.032185	1.304455	1.407357
C	0.069252	0.062262	0.719064
C	0.069252	0.062262	-0.719064
H	0.111240	-1.188662	2.485143
H	0.191550	-3.317580	1.245158
H	0.191550	-3.317580	-1.245158
H	0.111240	-1.188662	-2.485143
H	0.040487	1.306052	-2.488735
H	-0.005717	3.423268	-1.237901
H	-0.005717	3.423268	1.237901
H	0.040487	1.306052	2.488735

2-Na^+			PG: C_s
Na	-1.870007	-1.355110	0.000000
C	0.473725	-1.012585	1.402873
C	0.649721	-2.190588	0.709535
C	0.649721	-2.190588	-0.709535
C	0.473725	-1.012585	-1.402873
C	0.120255	1.452653	-1.404674
C	-0.035496	2.622564	-0.706943
C	-0.035496	2.622564	0.706943
C	0.120255	1.452653	1.404674
C	0.289003	0.222107	0.718040
C	0.289003	0.222107	-0.718040
H	0.500791	-1.010098	2.484823
H	0.817703	-3.114859	1.244643
H	0.817703	-3.114859	-1.244643
H	0.500791	-1.010098	-2.484823
H	0.134333	1.456686	-2.486319
H	-0.151031	3.556474	-1.238387
H	-0.151031	3.556474	1.238387
H	0.134333	1.456686	2.486319

2-K^+			PG: Cs
K	-1.841442	-1.524965	0.000000
C	0.899181	-0.756315	1.401289
C	1.270352	-1.885773	0.708390
C	1.270352	-1.885773	-0.708390
C	0.899181	-0.756315	-1.401289
C	0.123338	1.608535	-1.403181
C	-0.240631	2.732882	-0.706846
C	-0.240631	2.732882	0.706846
C	0.123338	1.608535	1.403181
C	0.505939	0.426524	0.716906
C	0.505939	0.426524	-0.716906
H	0.928858	-0.747767	2.483382
H	1.593845	-2.768116	1.243241
H	1.593845	-2.768116	-1.243241
H	0.928858	-0.747767	-2.483382
H	0.140516	1.616259	-2.485004
H	-0.518591	3.631670	-1.238893
H	-0.518591	3.631670	1.238893
H	0.140516	1.616259	2.485004

3			PG: C_{2v}
C	0.000000	2.829732	0.875660
C	0.000000	0.677227	2.088400
C	0.000000	1.419024	0.863555
C	0.000000	0.727298	-0.378864
C	0.000000	-0.727298	-0.378864
C	0.000000	-1.419024	0.863555
C	0.000000	3.550693	-0.296104
C	0.000000	2.873635	-1.525116
C	0.000000	1.495848	-1.561923
C	0.000000	-1.495848	-1.561923
C	0.000000	-2.873635	-1.525116
C	0.000000	-3.550693	-0.296104
C	0.000000	-2.829732	0.875660
C	0.000000	-0.677227	2.088400
H	0.000000	3.340190	1.830132
H	0.000000	1.225715	3.021407
H	0.000000	4.631729	-0.272134
H	0.000000	3.434537	-2.449739
H	0.000000	1.004942	-2.523316
H	0.000000	-1.004942	-2.523316
H	0.000000	-3.434537	-2.449739
H	0.000000	-4.631729	-0.272134
H	0.000000	-3.340190	1.830132
H	0.000000	-1.225715	3.021407

3-Li$^+$			PG: C_s
Li	-0.902600	1.734498	0.000000
C	-0.850042	-0.079838	2.844310
C	-0.836444	-0.076649	1.429199
C	-2.065082	-0.106977	0.682475
C	0.411856	-0.038761	0.731200
C	0.411856	-0.038761	-0.731200
C	-0.836444	-0.076649	-1.429199
C	0.323540	-0.057568	3.556060
C	1.553776	-0.018181	2.875813
C	1.598193	-0.003460	1.500932
C	1.598193	-0.003460	-1.500932
C	1.553776	-0.018181	-2.875813
C	0.323540	-0.057568	-3.556060
C	-0.850042	-0.079838	-2.844310
C	-2.065082	-0.106977	-0.682475
H	-1.801962	-0.117463	3.356375
H	-2.999356	-0.137505	1.226610
H	0.304956	-0.073501	4.636236
H	2.476012	-0.003284	3.439002
H	2.559466	0.018607	1.012002
H	2.559466	0.018607	-1.012002
H	2.476012	-0.003284	-3.439002
H	0.304956	-0.073501	-4.636236
H	-1.801962	-0.117463	-3.356375
H	-2.999356	-0.137505	-1.226610

3-Na$^+$			PG: C_s
Na	-1.030303	1.983807	0.000000
C	-0.748935	-0.355864	2.840095
C	-0.736700	-0.346323	1.426866
C	-1.953509	-0.521269	0.680668
C	0.498153	-0.169215	0.730941
C	0.498153	-0.169215	-0.730941
C	-0.736700	-0.346323	-1.426866
C	0.414610	-0.199580	3.556008
C	1.631409	-0.022393	2.877748
C	1.671984	-0.005114	1.500585
C	1.671984	-0.005114	-1.500585
C	1.631409	-0.022393	-2.877748
C	0.414610	-0.199580	-3.556008
C	-0.748935	-0.355864	-2.840095
C	-1.953509	-0.521269	-0.680668
H	-1.689937	-0.506023	3.352374
H	-2.874577	-0.679645	1.226053
H	0.395983	-0.220071	4.636197
H	2.547001	0.093827	3.440082
H	2.626128	0.119529	1.012310
H	2.626128	0.119529	-1.012310
H	2.547001	0.093827	-3.440082
H	0.395983	-0.220071	-4.636197
H	-1.689937	-0.506023	-3.352374
H	-2.874577	-0.679645	-1.226053

3-K$^+$			PG: C_s
K	-1.411476	1.956615	0.00000
C	-0.530044	-0.720944	2.836988
C	-0.516609	-0.718751	1.424042
C	-1.652942	-1.183370	0.679546
C	0.639459	-0.253904	0.729730
C	0.639459	-0.253904	-0.729730
C	-0.516609	-0.718751	-1.424042
C	0.557463	-0.279857	3.554876
C	1.697771	0.180593	2.877187
C	1.736928	0.193555	1.499308
C	1.736928	0.193555	-1.499308
C	1.697771	0.180593	-2.877187
C	0.557463	-0.279857	-3.554876
C	-0.530044	-0.720944	-2.836988
C	-1.652942	-1.183370	-0.679546
H	-1.407693	-1.092643	3.349163
H	-2.508230	-1.559388	1.225680
H	0.540131	-0.296041	4.635251
H	2.556909	0.518168	3.439440
H	2.635759	0.538137	1.011296
H	2.635759	0.538137	-1.011296
H	2.556909	0.518168	-3.439440
H	0.540131	-0.296041	-4.635251
H	-1.407693	-1.092643	-3.349163
H	-2.508230	-1.559388	-1.225680

4			PG: D_{3h}
C	0.708019	1.253801	0.000000
C	1.439833	-0.013738	0.000000
C	0.731814	-1.240063	0.000000
C	-0.731814	-1.240063	0.000000
C	-1.439833	-0.013738	0.000000
C	-0.708019	1.253801	0.000000
C	1.379626	2.492950	0.000000
C	-1.379626	2.492950	0.000000
C	0.698414	3.691065	0.000000
C	-0.698414	3.691065	0.000000
H	2.457418	2.520725	0.000000
H	-2.457418	2.520725	0.000000
H	1.245797	4.623570	0.000000
H	-1.245797	4.623570	0.000000
C	1.469145	-2.441266	0.000000
C	2.848771	-0.051684	0.000000
C	2.847349	-2.450377	0.000000
C	3.545763	-1.240689	0.000000
H	0.954303	-3.388549	0.000000
H	3.411720	0.867824	0.000000
H	4.627027	-1.232893	0.000000
H	3.381230	-3.390677	0.000000
C	-2.848771	-0.051684	0.000000
C	-1.469145	-2.441266	0.000000
C	-3.545763	-1.240689	0.000000
C	-2.847349	-2.450377	0.000000
H	-3.411720	0.867824	0.000000
H	-0.954303	-3.388549	0.000000
H	-4.627027	-1.232893	0.000000
H	-3.381230	-3.390677	0.000000

4-Li$^+$			PG: C_{3v}
Li	0.000000	0.000000	1.757841
C	0.712132	1.260404	-0.044995
C	1.447608	-0.013478	-0.044995
C	0.735476	-1.246927	-0.044995
C	-0.735476	-1.246927	-0.044995
C	-1.447608	-0.013478	-0.044995
C	-0.712132	1.260404	-0.044995
C	1.386078	2.503469	-0.039441
C	-1.386078	2.503469	-0.039441
C	0.700026	3.695374	-0.045334
C	-0.700026	3.695374	-0.045334
H	2.463255	2.532749	-0.046769
H	-2.463255	2.532749	-0.046769
H	1.243707	4.629122	-0.053531
H	-1.243707	4.629122	-0.053531
C	1.475028	-2.452113	-0.039441
C	2.861107	-0.051355	-0.039441
C	2.850275	-2.453928	-0.045334
C	3.550301	-1.241447	-0.045334
H	0.961797	-3.399616	-0.046769
H	3.425053	0.866867	-0.046769
H	4.630791	-1.237479	-0.053531
H	3.387084	-3.391643	-0.053531
C	-2.861107	-0.051355	-0.039441
C	-1.475028	-2.452113	-0.039441
C	-3.550301	-1.241447	-0.045334
C	-2.850275	-2.453928	-0.045334
H	-3.425053	0.866867	-0.046769
H	-0.961797	-3.399616	-0.046769
H	-4.630791	-1.237479	-0.053531
H	-3.387084	-3.391643	-0.053531

4-Na$^+$			PG: C_{3v}
Na	0.000000	0.000000	2.141293
C	0.711099	1.259578	-0.192599
C	1.446376	-0.013959	-0.192599
C	0.735277	-1.245618	-0.192599
C	-0.735277	-1.245618	-0.192599
C	-1.446376	-0.013959	-0.192599
C	-0.711099	1.259578	-0.192599
C	1.384014	2.501105	-0.193200
C	-1.384014	2.501105	-0.193200
C	0.699044	3.696292	-0.199129
C	-0.699044	3.696292	-0.199129
H	2.461448	2.530978	-0.205264
H	-2.461448	2.530978	-0.205264
H	1.244095	4.629299	-0.210869
H	-1.244095	4.629299	-0.210869
C	1.474013	-2.449143	-0.193200
C	2.858027	-0.051961	-0.193200
C	2.851561	-2.453536	-0.199129
C	3.550605	-1.242757	-0.199129
H	0.961167	-3.397166	-0.205264
H	3.422615	0.866188	-0.205264
H	4.631138	-1.237232	-0.210869
H	3.387043	-3.392067	-0.210869
C	-2.858027	-0.051961	-0.193200
C	-1.474013	-2.449143	-0.193200
C	-3.550605	-1.242757	-0.199129
C	-2.851561	-2.453536	-0.199129
H	-3.422615	0.866188	-0.205264
H	-0.961167	-3.397166	-0.205264
H	-4.631138	-1.237232	-0.210869
H	-3.387043	-3.392067	-0.210869

4-K$^+$			PG: C_{3v}
K	0.000000	0.000000	2.418039
C	0.710074	1.257516	-0.384813
C	1.444078	-0.013816	-0.384813
C	0.734004	-1.243700	-0.384813
C	-0.734004	-1.243700	-0.384813
C	-1.444078	-0.013816	-0.384813
C	-0.710074	1.257516	-0.384813
C	1.382975	2.498816	-0.381104
C	-1.382975	2.498816	-0.381104
C	0.698947	3.695180	-0.379650
C	-0.698947	3.695180	-0.379650
H	2.460486	2.528855	-0.395715
H	-2.460486	2.528855	-0.395715
H	1.244447	4.628046	-0.388011
H	-1.244447	4.628046	-0.388011
C	1.472550	-2.447099	-0.381104
C	2.855525	-0.051716	-0.381104
C	2.850646	-2.452896	-0.379650
C	3.549593	-1.242284	-0.379650
H	0.959810	-3.395271	-0.395715
H	3.420296	0.866416	-0.395715
H	4.630230	-1.236300	-0.388011
H	3.385782	-3.391746	-0.388011
C	-2.855525	-0.051716	-0.381104
C	-1.472550	-2.447099	-0.381104
C	-3.549593	-1.242284	-0.379650
C	-2.850646	-2.452896	-0.379650
H	-3.420296	0.866416	-0.395715
H	-0.959810	-3.395271	-0.395715
H	-4.630230	-1.236300	-0.388011
H	-3.385782	-3.391746	-0.388011

5			PG: C_s
C	-0.701265	-0.070308	0.000000
C	-1.590061	0.980104	0.000000
C	-1.064404	2.284332	0.000000
C	0.306084	2.501491	0.000000
C	1.209366	1.423703	0.000000
C	0.688985	0.150004	0.000000
C	-0.794998	-1.586184	0.000000
C	1.246377	-1.263100	0.000000
C	0.306084	-1.932729	1.062662
C	0.306084	-1.932729	-1.062662
H	0.475847	-3.004777	1.157499
H	0.231665	-1.462451	2.041503
H	0.475847	-3.004777	-1.157499
H	0.231665	-1.462451	-2.041503
H	2.322389	-1.406934	0.000000
H	-1.774007	-2.055201	0.000000
H	-1.738473	3.130224	0.000000
H	-2.660580	0.821049	0.000000
H	2.276594	1.603462	0.000000
H	0.685550	3.514349	0.000000

5-Li$^+$			PG: C_s
Li	1.695333	1.361130	0.000000
C	-0.038204	-0.025806	0.709668
C	-0.099535	1.159436	1.423184
C	-0.172809	2.371783	0.697646
C	-0.172809	2.371783	-0.697646
C	-0.099535	1.159436	-1.423184
C	-0.038204	-0.025806	-0.709668
C	-0.019808	-1.503026	1.039814
C	-0.019808	-1.503026	-1.039814
C	1.035630	-2.016292	0.000000
C	-1.086494	-2.010558	0.000000
H	1.121912	-3.099418	0.000000
H	2.028947	-1.563211	0.000000
H	-1.176690	-3.093487	0.000000
H	-2.065872	-1.538642	0.000000
H	-0.019340	-1.809890	-2.079115
H	-0.019340	-1.809890	2.079115
H	-0.234416	3.309242	1.232016
H	-0.108665	1.172553	2.504651
H	-0.108665	1.172553	-2.504651
H	-0.234416	3.309242	-1.232016

5-Na$^+$			PG: C_s
Na	-2.085887	-1.178548	0.000000
C	0.277555	0.152705	0.708452
C	0.271983	-1.031104	1.422257
C	0.271983	-2.244381	0.696703
C	0.271983	-2.244381	-0.696703
C	0.271983	-1.031104	-1.422257
C	0.277555	0.152705	-0.708452
C	0.368487	1.628839	1.038616
C	0.368487	1.628839	-1.038616
C	-0.645475	2.219658	0.000000
C	1.468518	2.059802	0.000000
H	-0.658021	3.306490	0.000000
H	-1.670767	1.839882	0.000000
H	1.640552	3.133180	0.000000
H	2.409756	1.515833	0.000000
H	0.391159	1.937237	-2.077543
H	0.391159	1.937237	2.077543
H	0.304872	-3.183969	1.230833
H	0.306412	-1.043679	2.503538
H	0.306412	-1.043679	-2.503538
H	0.304872	-3.183969	-1.230833

5-K$^+$			PG: C_s
K	-2.277376	-1.111358	0.000000
C	0.563508	0.267223	0.707107
C	0.560438	-0.914736	1.420477
C	0.560438	-2.125940	0.695789
C	0.560438	-2.125940	-0.695789
C	0.560438	-0.914736	-1.420477
C	0.563508	0.267223	-0.707107
C	0.660312	1.744209	1.037852
C	0.660312	1.744209	-1.037852
C	-0.350808	2.340972	0.000000
C	1.761890	2.172488	0.000000
H	-0.357315	3.428062	0.000000
H	-1.377849	1.966826	0.000000
H	1.938841	3.245318	0.000000
H	2.699969	1.623204	0.000000
H	0.684518	2.053730	-2.076641
H	0.684518	2.053730	2.076641
H	0.598020	-3.065723	1.229951
H	0.599296	-0.926723	2.501882
H	0.599296	-0.926723	-2.501882
H	0.598020	-3.065723	-1.229951

6			PG: C_{2v}
C	0.000000	1.369926	0.884751
C	0.000000	0.710423	2.087351
C	0.000000	-0.710423	2.087351
C	0.000000	-1.369926	0.884751
C	0.000000	-0.681133	-0.359410
C	0.000000	0.681133	-0.359410
C	0.000000	2.822803	0.443592
C	0.000000	1.819268	-1.364922
C	-1.062259	2.770131	-0.709568
C	1.062259	2.770131	-0.709568
H	-1.157112	3.718538	-1.237616
H	-2.041256	2.354295	-0.478140
H	1.157112	3.718538	-1.237616
H	2.041256	2.354295	-0.478140
H	0.000000	1.591035	-2.426039
H	0.000000	3.602629	1.198875
C	0.000000	-1.819268	-1.364922
C	0.000000	-2.822803	0.443592
C	-1.062259	-2.770131	-0.709568
C	1.062259	-2.770131	-0.709568
H	-1.157112	-3.718538	-1.237616
H	-2.041256	-2.354295	-0.478140
H	1.157112	-3.718538	-1.237616
H	2.041256	-2.354295	-0.478140
H	0.000000	-3.602629	1.198875
H	0.000000	-1.591035	-2.426039
H	0.000000	-1.250116	3.025329
H	0.000000	1.250116	3.025329

6-Li$^+$			PG: C_s
Li	-1.082445	1.694954	0.000000
C	-0.855373	-0.072734	1.383633
C	-2.059301	-0.173847	0.715299
C	-2.059301	-0.173847	-0.715299
C	-0.855373	-0.072734	-1.383633
C	0.392185	0.037361	-0.685963
C	0.392185	0.037361	0.685963
C	-0.409440	-0.103956	2.831399
C	1.399183	0.052509	1.818169
C	0.685276	1.017602	2.825767
C	0.803764	-1.097305	2.710949
H	1.211167	1.086645	3.774307
H	0.406859	2.015659	2.481444
H	1.339991	-1.208164	3.649805
H	0.627369	-2.065095	2.247935
H	2.454681	0.126568	1.584720
H	-1.159740	-0.186893	3.609091
C	1.399183	0.052509	-1.818169
C	-0.409440	-0.103956	-2.831399
C	0.685276	1.017602	-2.825767
C	0.803764	-1.097305	-2.710949
H	1.211167	1.086645	-3.774307
H	0.406859	2.015659	-2.481444
H	1.339991	-1.208164	-3.649805
H	0.627369	-2.065095	-2.247935
H	-1.159740	-0.186893	-3.609091
H	2.454681	0.126568	-1.584720
H	-2.994430	-0.268938	-1.249891
H	-2.994430	-0.268938	1.249891

6-Na$^+$			PG: C_s
Na	-1.743069	1.571639	0.000000
C	-0.637716	-0.487253	1.380311
C	-1.730540	-0.999404	0.714903
C	-1.730540	-0.999404	-0.714903
C	-0.637716	-0.487253	-1.380311
C	0.495263	0.043735	-0.684511
C	0.495263	0.043735	0.684511
C	-0.201432	-0.380396	2.828343
C	1.443542	0.386205	1.817421
C	0.451671	1.044154	2.835981
C	1.275888	-0.902968	2.701086
H	0.924700	1.282232	3.785304
H	-0.148380	1.894937	2.500939
H	1.821573	-0.836171	3.639197
H	1.434365	-1.868942	2.228099
H	2.412112	0.814405	1.586828
H	-0.874791	-0.719080	3.607578
C	1.443542	0.386205	-1.817421
C	-0.201432	-0.380396	-2.828343
C	0.451671	1.044154	-2.835981
C	1.275888	-0.902968	-2.701086
H	0.924700	1.282232	-3.785304
H	-0.148380	1.894937	-2.500939
H	1.821573	-0.836171	-3.639197
H	1.434365	-1.868942	-2.228099
H	-0.874791	-0.719080	-3.607578
H	2.412112	0.814405	-1.586828
H	-2.562761	-1.435835	-1.250895
H	-2.562761	-1.435835	1.250895

6-K$^+$			PG: C_s
K	2.450327	-0.814985	0.000000
C	0.142290	0.798416	1.377421
C	0.895975	1.739587	0.713509
C	0.895975	1.739587	-0.713509
C	0.142290	0.798416	-1.377421
C	-0.640657	-0.174800	-0.683654
C	-0.640657	-0.174800	0.683654
C	-0.209732	0.517033	2.826346
C	-1.348733	-0.894480	1.816530
C	-0.174779	-1.049280	2.842251
C	-1.766190	0.340617	2.694859
H	-0.500992	-1.466310	3.791905
H	0.737833	-1.554541	2.514447
H	-2.232678	0.045643	3.632012
H	-2.328020	1.138326	2.215338
H	-2.032270	-1.704011	1.587214
H	0.243327	1.119146	3.606175
C	-1.348733	-0.894480	-1.816530
C	-0.209732	0.517033	-2.826346
C	-0.174779	-1.049280	-2.842251
C	-1.766190	0.340617	-2.694859
H	-0.500992	-1.466310	-3.791905
H	0.737833	-1.554541	-2.514447
H	-2.232678	0.045643	-3.632012
H	-2.328020	1.138326	-2.215338
H	0.243327	1.119146	-3.606175
H	-2.032270	-1.704011	-1.587214
H	1.445644	2.501555	-1.250519
H	1.445644	2.501555	1.250519

7			PG: D_{3h}
C	-0.678964	1.221701	0.000000
C	0.678964	1.221701	0.000000
C	1.397506	-0.022851	0.000000
C	0.718542	-1.198850	0.000000
C	-0.718542	-1.198850	0.000000
C	-1.397506	-0.022851	0.000000
C	-1.806351	2.238144	0.000000
C	-2.841466	0.445274	0.000000
C	-2.767554	1.597848	1.062040
C	-2.767554	1.597848	-1.062040
H	-3.707659	2.140618	1.157178
H	-2.355243	1.359800	2.041012
H	-3.707659	2.140618	-1.157178
H	-2.355243	1.359800	-2.041012
H	-3.637729	-0.291942	0.000000
H	-1.566035	3.296336	0.000000
C	2.841466	0.445274	0.000000
C	1.806351	2.238144	0.000000
C	2.767554	1.597848	1.062040
C	2.767554	1.597848	-1.062040
H	3.707659	2.140618	1.157178
H	2.355243	1.359800	2.041012
H	3.707659	2.140618	-1.157178
H	2.355243	1.359800	-2.041012
H	1.566035	3.296336	0.000000
H	3.637729	-0.291942	0.000000
C	-1.035114	-2.683418	0.000000
C	1.035114	-2.683418	0.000000
C	0.000000	-3.195696	1.062040
C	0.000000	-3.195696	-1.062040
H	0.000000	-4.281236	1.157178
H	0.000000	-2.719601	2.041012
H	0.000000	-4.281236	-1.157178
H	0.000000	-2.719601	-2.041012
H	2.071693	-3.004395	0.000000
H	-2.071693	-3.004395	0.000000

7-Li$^+$			PG: C_{3v}
Li	0.000000	0.000000	1.787481
C	-0.684131	1.231906	0.033297
C	0.684131	1.231906	0.033297
C	1.408928	-0.023478	0.033297
C	0.724796	-1.208428	0.033297
C	-0.724796	-1.208428	0.033297
C	-1.408928	-0.023478	0.033297
C	-1.809682	2.244522	-0.048725
C	-2.848655	0.444970	-0.048725
C	-2.831523	1.634781	0.970401
C	-2.704346	1.561355	-1.144520
H	-3.772687	2.178162	0.988252
H	-2.495584	1.440826	1.991219
H	-3.634824	2.098567	-1.309981
H	-2.239340	1.292884	-2.090062
H	-3.639857	-0.295150	-0.068530
H	-1.564321	3.299784	-0.068530
C	2.848655	0.444970	-0.048725
C	1.809682	2.244522	-0.048725
C	2.831523	1.634781	0.970401
C	2.704346	1.561355	-1.144520
H	3.772687	2.178162	0.988252
H	2.495584	1.440826	1.991219
H	3.634824	2.098567	-1.309981
H	2.239340	1.292884	-2.090062
H	1.564321	3.299784	-0.068530
H	3.639857	-0.295150	-0.068530
C	-1.038972	-2.689492	-0.048725
C	1.038972	-2.689492	-0.048725
C	0.000000	-3.269561	0.970401
C	0.000000	-3.122709	-1.144520
H	0.000000	-4.356324	0.988252
H	0.000000	-2.881652	1.991219
H	0.000000	-4.197133	-1.309981
H	0.000000	-2.585767	-2.090062
H	2.075536	-3.004633	-0.068530
H	-2.075536	-3.004633	-0.068530

7-Na$^+$			PG: C_{3v}
Na	0.000000	0.000000	2.212837
C	-0.682444	1.230333	-0.095213
C	0.682444	1.230333	-0.095213
C	1.406722	-0.024152	-0.095213
C	0.724278	-1.206181	-0.095213
C	-0.724278	-1.206181	-0.095213
C	-1.406722	-0.024152	-0.095213
C	-1.807059	2.242643	-0.202861
C	-2.845715	0.443638	-0.202861
C	-2.845489	1.642844	0.805292
C	-2.688354	1.552122	-1.304625
H	-3.786953	2.186398	0.807578
H	-2.525742	1.458238	1.834907
H	-3.616504	2.087989	-1.488550
H	-2.208448	1.275048	-2.239948
H	-3.639115	-0.294584	-0.227413
H	-1.564440	3.298858	-0.227413
C	2.845715	0.443638	-0.202861
C	1.807059	2.242643	-0.202861
C	2.845489	1.642844	0.805292
C	2.688354	1.552122	-1.304625
H	3.786953	2.186398	0.807578
H	2.525742	1.458238	1.834907
H	3.616504	2.087989	-1.488550
H	2.208448	1.275048	-2.239948
H	1.564440	3.298858	-0.227413
H	3.639115	-0.294584	-0.227413
C	-1.038656	-2.686280	-0.202861
C	1.038656	-2.686280	-0.202861
C	0.000000	-3.285687	0.805292
C	0.000000	-3.104244	-1.304625
H	0.000000	-4.372797	0.807578
H	0.000000	-2.916476	1.834907
H	0.000000	-4.175979	-1.488550
H	0.000000	-2.550096	-2.239948
H	2.074675	-3.004274	-0.227413
H	-2.074675	-3.004274	-0.227413

7-K$^+$		PG: C_{3v}	
K	0.000000	0.000000	2.512213
C	-0.681574	1.227899	-0.268578
C	0.681574	1.227899	-0.268578
C	1.404179	-0.023689	-0.268578
C	0.722604	-1.204210	-0.268578
C	-0.722604	-1.204210	-0.268578
C	-1.404179	-0.023689	-0.268578
C	-1.805739	2.241134	-0.389979
C	-2.843749	0.443249	-0.389979
C	-2.854425	1.648003	0.611484
C	-2.678377	1.546362	-1.495496
H	-3.796072	2.191663	0.600379
H	-2.547617	1.470868	1.646074
H	-3.604992	2.081343	-1.691267
H	-2.189078	1.263865	-2.424329
H	-3.637406	-0.294946	-0.417393
H	-1.563273	3.297559	-0.417393
C	2.843749	0.443249	-0.389979
C	1.805739	2.241134	-0.389979
C	2.854425	1.648003	0.611484
C	2.678377	1.546362	-1.495496
H	3.796072	2.191663	0.600379
H	2.547617	1.470868	1.646074
H	3.604992	2.081343	-1.691267
H	2.189078	1.263865	-2.424329
H	1.563273	3.297559	-0.417393
H	3.637406	-0.294946	-0.417393
C	-1.038010	-2.684383	-0.389979
C	1.038010	-2.684383	-0.389979
C	0.000000	-3.296006	0.611484
C	0.000000	-3.092724	-1.495496
H	0.000000	-4.383327	0.600379
H	0.000000	-2.941735	1.646074
H	0.000000	-4.162686	-1.691267
H	0.000000	-2.527730	-2.424329
H	2.074134	-3.002614	-0.417393
H	-2.074134	-3.002614	-0.417393

Table S2: Total energies, BSSE corrections, and zero-point vibrational energy (ZPVE) corrections, obtained at the B3LYP/6-311+G(2d,2p) level. All values are in hartrees.[a]

System		Ligand	Ligand-Li^+	Ligand-Na^+	Ligand-K^+
1	Energy	-232.32067	-239.66742	-394.44707	-832.10767
	BSSE correction		0.00062	0.00065	0.00038
	ZPVE	0.10033	0.10318	0.10180	0.10151
2	Energy	-386.00394	-393.35480	-548.13388	-985.79422
	BSSE correction		0.00064	0.00119	0.0005
	ZPVE	0.14714	0.14990	0.14847	0.14820
3	Energy	-539.68916	-547.04153	-701.82132	-1139.48177
	BSSE correction		0.00064	0.00116	0.0005
	ZPVE	0.19399	0.19656	0.19523	0.19500
4	Energy	-693.37104	-700.72383	-855.50492	-1293.16545
	BSSE correction		0.00068	0.00124	0.00053
	ZPVE	0.24107	0.24341	0.24220	0.24194
5	Energy	-387.14271	-394.49996	-549.27648	-986.93511
	BSSE correction		0.00059	0.00117	0.00044
	ZPVE	0.17017	0.17319	0.17163	0.17132
6	Energy	-541.96441	-549.33000	-704.10396	-1141.76090
	BSSE correction		0.00061	0.00123	0.00052
	ZPVE	0.23990	0.24307	0.24136	0.24100
7	Energy	-696.78598	-704.158337	-858.93002	-1296.58545
	BSSE correction		0.00066	0.00129	0.00052
	ZPVE	0.30967	0.31297	0.31109	0.31074

(a) Energies of metal ions: $E_{Li^+} = -7.28492$; $E_{Na^+} = -162.08757$; $E_{K^+} = -599.76105$ hartrees

Table S3: B3LYP/6-311+G(2d,2p) level unscaled vibrational frequencies (in cm^{-1}) for ligands **1**-**7** and their complexes with the alkali metal ions. The intensities (in km/mol) are given in parentheses.

No.	**1**		**1-Li$^+$**		**1-Na$^+$**		**1-K$^+$**	
1	410	(0)	270	(11)	115	(2)	97	(0)
2	410	(0)	270	(11)	115	(2)	97	(0)
3	624	(0)	383	(101)	194	(35)	131	(23)
4	624	(0)	416	(0)	417	(0)	414	(0)
5	683	(115)	416	(0)	417	(0)	414	(0)
6	717	(0)	623	(0)	622	(0)	622	(0)
7	861	(0)	623	(0)	622	(0)	622	(0)
8	861	(0)	713	(0)	717	(0)	715	(0)
9	989	(0)	752	(144)	736	(126)	725	(122)
10	989	(0)	918	(1)	904	(1)	896	(1)
11	1012	(0)	918	(1)	904	(1)	896	(1)
12	1016	(0)	997	(1)	998	(2)	1002	(2)
13	1031	(0)	1031	(0)	1021	(0)	1016	(0)
14	1060	(5)	1031	(0)	1021	(0)	1016	(0)
15	1060	(5)	1035	(0)	1027	(0)	1024	(0)
16	1176	(0)	1051	(3)	1048	(0)	1045	(0)
17	1200	(0)	1051	(3)	1052	(4)	1055	(4)
18	1200	(0)	1054	(0)	1052	(4)	1055	(4)
19	1332	(0)	1187	(0)	1182	(0)	1181	(0)
20	1391	(0)	1204	(0)	1203	(0)	1203	(0)
21	1519	(7)	1204	(0)	1203	(0)	1203	(0)
22	1519	(7)	1316	(0)	1316	(0)	1324	(0)
23	1634	(0)	1393	(0)	1394	(0)	1394	(0)
24	1634	(0)	1510	(19)	1512	(15)	1515	(13)
25	3164	(0)	1510	(19)	1512	(15)	1515	(13)
26	3173	(0)	1608	(0)	1615	(0)	1620	(0)
27	3173	(0)	1608	(0)	1615	(0)	1620	(0)
28	3188	(35)	3188	(0)	3180	(0)	3176	(0)
29	3188	(35)	3195	(0)	3187	(0)	3184	(0)
30	3199	(0)	3195	(0)	3187	(0)	3184	(0)
31			3205	(4)	3198	(0)	3196	(1)
32			3205	(4)	3198	(0)	3196	(1)
33			3211	(0)	3205	(0)	3204	(0)

No.	**2**		**2-Li$^+$**		**2-Na$^+$**		**2-K$^+$**	
1	172	(3)	153	(10)	70	(8)	49	(4)
2	185	(0)	164	(6)	90	(4)	74	(1)
3	366	(2)	262	(15)	185	(1)	132	(22)
4	396	(0)	277	(8)	193	(0)	188	(8)
5	478	(0)	366	(2)	197	(41)	193	(0)
6	488	(22)	385	(63)	365	(1)	365	(1)
7	520	(0)	405	(32)	396	(0)	396	(0)
8	520	(0)	475	(0)	476	(0)	476	(0)
9	635	(0)	502	(42)	496	(25)	496	(24)
10	637	(3)	519	(0)	518	(0)	518	(0)
11	728	(0)	520	(0)	518	(0)	518	(0)
12	773	(0)	630	(0)	632	(0)	633	(0)
13	786	(0)	634	(2)	633	(2)	634	(2)
14	798	(119)	763	(3)	757	(2)	753	(1)
15	811	(0)	765	(1)	765	(0)	766	(0)
16	851	(0)	787	(0)	786	(0)	787	(0)
17	900	(0)	808	(0)	807	(0)	807	(0)
18	956	(0)	837	(127)	827	(123)	822	(120)
19	966	(0)	883	(0)	875	(0)	873	(0)
20	987	(4)	928	(1)	918	(1)	916	(1)
21	999	(0)	957	(0)	954	(0)	954	(0)
22	1004	(0)	996	(0)	989	(1)	987	(1)
23	1033	(9)	1013	(4)	1007	(4)	1004	(4)
24	1044	(0)	1025	(0)	1018	(0)	1017	(0)
25	1154	(5)	1027	(3)	1026	(5)	1025	(0)
26	1168	(1)	1034	(0)	1029	(0)	1029	(5)
27	1173	(0)	1040	(0)	1042	(0)	1042	(0)
28	1188	(0)	1155	(3)	1154	(4)	1155	(4)
29	1231	(1)	1178	(0)	1173	(0)	1173	(0)
30	1274	(0)	1179	(0)	1176	(0)	1176	(0)
31	1291	(6)	1197	(1)	1195	(0)	1194	(0)
32	1389	(1)	1231	(1)	1230	(1)	1231	(1)
33	1391	(0)	1274	(0)	1274	(0)	1275	(0)
34	1426	(4)	1291	(10)	1290	(9)	1291	(9)
35	1495	(0)	1368	(8)	1372	(4)	1379	(3)
36	1497	(0)	1395	(27)	1389	(15)	1389	(9)
37	1549	(8)	1426	(7)	1426	(6)	1427	(6)
38	1610	(0)	1489	(0)	1490	(0)	1491	(0)
39	1637	(3)	1494	(1)	1494	(1)	1496	(0)
40	1665	(0)	1536	(16)	1540	(15)	1543	(14)

41	3163	(0)	1596	(2)	1598	(1)	1601	(1)
42	3165	(5)	1618	(6)	1624	(6)	1629	(6)
43	3167	(1)	1653	(3)	1654	(2)	1656	(1)
44	3171	(0)	3184	(0)	3176	(0)	3172	(0)
45	3181	(0)	3186	(0)	3179	(0)	3175	(0)
46	3182	(51)	3186	(0)	3181	(1)	3178	(1)
47	3193	(37)	3190	(0)	3184	(0)	3181	(0)
48	3194	(0)	3199	(0)	3192	(1)	3188	(2)
49			3201	(1)	3197	(2)	3195	(4)
50			3208	(2)	3202	(0)	3199	(1)
51			3210	(0)	3208	(0)	3206	(1)

No.	**3**		**3-Li$^+$**		**3-Na$^+$**		**3-K$^+$**	
1	96	(0)	96	(2)	57	(9)	37	(5)
2	100	(1)	99	(0)	76	(8)	55	(3)
3	228	(4)	183	(13)	95	(0)	90	(2)
4	242	(0)	188	(16)	99	(0)	97	(0)
5	248	(0)	245	(1)	194	(38)	140	(26)
6	400	(0)	267	(4)	234	(8)	236	(7)
7	412	(1)	283	(15)	244	(0)	246	(0)
8	436	(8)	379	(75)	247	(1)	247	(1)
9	447	(2)	405	(1)	403	(1)	402	(0)
10	506	(1)	411	(1)	410	(1)	411	(1)
11	507	(5)	447	(1)	438	(11)	438	(10)
12	544	(0)	448	(47)	446	(1)	446	(1)
13	558	(0)	500	(13)	501	(6)	503	(6)
14	602	(0)	503	(2)	504	(1)	505	(1)
15	634	(5)	548	(1)	547	(1)	547	(1)
16	724	(0)	556	(0)	555	(0)	556	(0)
17	728	(1)	591	(1)	594	(0)	596	(0)
18	728	(2)	631	(3)	631	(3)	632	(3)
19	747	(87)	717	(0)	717	(0)	719	(0)
20	769	(0)	724	(2)	724	(2)	725	(2)
21	805	(0)	738	(10)	735	(7)	734	(6)
22	829	(55)	767	(70)	766	(75)	764	(77)
23	845	(0)	780	(0)	780	(0)	780	(0)
24	885	(12)	805	(0)	804	(0)	805	(0)
25	885	(0)	838	(1)	839	(0)	841	(0)
26	890	(2)	859	(51)	852	(57)	849	(56)
27	965	(0)	885	(0)	884	(0)	886	(0)
28	973	(3)	894	(0)	892	(0)	891	(0)
29	989	(0)	904	(18)	902	(12)	900	(12)

30	1000	(0)	990	(0)	987	(0)	983	(0)
31	1002	(0)	998	(2)	995	(2)	991	(3)
32	1020	(3)	1010	(2)	1006	(2)	1005	(1)
33	1060	(2)	1015	(0)	1016	(0)	1017	(0)
34	1061	(6)	1028	(0)	1025	(0)	1022	(0)
35	1117	(2)	1030	(0)	1027	(0)	1023	(0)
36	1167	(2)	1057	(0)	1059	(0)	1059	(1)
37	1173	(0)	1059	(2)	1060	(2)	1061	(3)
38	1187	(0)	1118	(1)	1118	(1)	1118	(1)
39	1192	(0)	1176	(3)	1173	(3)	1172	(3)
40	1223	(1)	1180	(0)	1178	(0)	1178	(0)
41	1243	(0)	1187	(0)	1186	(0)	1188	(0)
42	1267	(9)	1204	(0)	1202	(0)	1200	(0)
43	1310	(0)	1225	(3)	1224	(3)	1224	(2)
44	1326	(2)	1239	(2)	1239	(2)	1241	(1)
45	1362	(0)	1267	(7)	1266	(8)	1267	(8)
46	1370	(1)	1313	(0)	1311	(0)	1311	(0)
47	1451	(1)	1320	(4)	1319	(3)	1322	(4)
48	1452	(1)	1361	(29)	1357	(13)	1357	(7)
49	1475	(4)	1361	(8)	1360	(5)	1363	(4)
50	1496	(10)	1442	(1)	1443	(0)	1446	(1)
51	1537	(6)	1450	(1)	1451	(1)	1452	(1)
52	1563	(2)	1472	(7)	1472	(6)	1473	(6)
53	1605	(0)	1495	(28)	1495	(21)	1495	(19)
54	1640	(2)	1528	(4)	1530	(6)	1533	(6)
55	1651	(0)	1556	(5)	1559	(4)	1560	(4)
56	1656	(0)	1596	(3)	1598	(2)	1599	(1)
57	3162	(0)	1625	(4)	1632	(5)	1635	(8)
58	3166	(2)	1642	(8)	1641	(4)	1644	(1)
59	3167	(2)	1650	(0)	1648	(0)	1648	(0)
60	3175	(0)	3181	(2)	3174	(1)	3171	(0)
61	3176	(12)	3185	(1)	3180	(1)	3178	(1)
62	3182	(32)	3186	(0)	3181	(0)	3179	(1)
63	3190	(38)	3194	(0)	3189	(1)	3187	(3)
64	3192	(1)	3195	(0)	3191	(0)	3188	(0)
65	3200	(9)	3196	(1)	3193	(2)	3191	(3)
66	3213	(17)	3207	(1)	3203	(2)	3200	(3)
67			3209	(0)	3206	(0)	3204	(0)
68			3215	(0)	3210	(1)	3208	(2)
69			3227	(1)	3221	(2)	3219	(4)

No.	**4**	**4-Li$^+$**	**4-Na$^+$**	**4-K$^+$**
1	53 (0)	57 (1)	49 (4)	36 (5)
2	53 (0)	57 (1)	49 (4)	36 (5)
3	111 (0)	114 (0)	69 (6)	58 (0)
4	121 (3)	119 (0)	69 (6)	58 (0)
5	262 (0)	188 (24)	110 (0)	95 (5)
6	262 (0)	188 (24)	112 (0)	113 (0)
7	272 (0)	260 (0)	197 (46)	153 (30)
8	272 (0)	260 (0)	260 (0)	261 (0)
9	411 (1)	280 (4)	260 (0)	261 (0)
10	411 (1)	280 (4)	272 (0)	272 (0)
11	421 (0)	364 (79)	272 (0)	272 (0)
12	431 (6)	410 (0)	410 (1)	410 (1)
13	434 (0)	410 (0)	410 (1)	410 (1)
14	434 (0)	418 (0)	418 (0)	419 (0)
15	553 (0)	439 (0)	434 (11)	433 (9)
16	553 (0)	439 (0)	436 (0)	437 (0)
17	568 (0)	447 (56)	436 (0)	437 (0)
18	582 (0)	548 (1)	545 (1)	543 (0)
19	621 (0)	548 (1)	545 (1)	543 (0)
20	638 (5)	565 (0)	567 (0)	567 (0)
21	638 (5)	567 (0)	570 (0)	573 (0)
22	713 (0)	618 (0)	619 (0)	619 (0)
23	726 (0)	635 (3)	635 (3)	636 (3)
24	726 (0)	635 (3)	635 (3)	636 (3)
25	752 (189)	707 (0)	708 (0)	709 (0)
26	789 (0)	730 (0)	730 (0)	730 (0)
27	789 (0)	730 (0)	730 (0)	730 (0)
28	790 (0)	768 (168)	768 (176)	767 (179)
29	791 (0)	782 (0)	782 (0)	786 (0)
30	791 (0)	782 (0)	784 (0)	786 (0)
31	871 (0)	783 (0)	784 (0)	789 (0)
32	871 (0)	797 (1)	795 (1)	794 (1)
33	892 (0)	797 (1)	795 (1)	794 (1)
34	963 (0)	884 (0)	883 (0)	882 (0)
35	963 (0)	884 (0)	884 (0)	882 (0)
36	971 (1)	888 (0)	884 (0)	886 (0)
37	994 (0)	986 (0)	982 (0)	979 (0)
38	1000 (0)	986 (0)	982 (0)	979 (0)
39	1000 (0)	994 (0)	990 (1)	988 (1)
40	1019 (4)	1012 (0)	1014 (0)	1014 (0)
41	1019 (4)	1012 (0)	1014 (0)	1015 (0)
42	1029 (0)	1021 (0)	1017 (0)	1015 (0)

43	1077	(6)	1026	(0)	1022	(0)	1020	(0)
44	1077	(6)	1026	(0)	1022	(0)	1020	(0)
45	1085	(0)	1026	(0)	1027	(0)	1028	(0)
46	1135	(0)	1074	(2)	1076	(3)	1076	(3)
47	1135	(0)	1074	(2)	1076	(3)	1076	(3)
48	1172	(0)	1081	(0)	1084	(0)	1084	(0)
49	1196	(0)	1135	(3)	1134	(2)	1134	(2)
50	1196	(0)	1135	(3)	1134	(2)	1134	(2)
51	1208	(0)	1181	(0)	1178	(0)	1176	(0)
52	1242	(0)	1206	(0)	1204	(0)	1203	(0)
53	1272	(5)	1206	(0)	1204	(0)	1203	(0)
54	1272	(5)	1214	(0)	1213	(0)	1212	(0)
55	1317	(0)	1239	(0)	1240	(0)	1241	(0)
56	1317	(0)	1272	(1)	1272	(2)	1272	(3)
57	1327	(0)	1272	(1)	1272	(2)	1272	(3)
58	1354	(0)	1310	(1)	1310	(0)	1312	(0)
59	1367	(0)	1310	(1)	1310	(0)	1312	(0)
60	1367	(0)	1329	(0)	1329	(0)	1328	(0)
61	1472	(20)	1339	(0)	1340	(0)	1345	(0)
62	1472	(20)	1363	(11)	1361	(6)	1363	(4)
63	1479	(0)	1363	(11)	1361	(6)	1363	(4)
64	1496	(0)	1471	(32)	1471	(28)	1472	(27)
65	1536	(10)	1471	(32)	1471	(28)	1472	(27)
66	1536	(10)	1472	(0)	1473	(0)	1475	(0)
67	1587	(0)	1496	(0)	1496	(0)	1496	(0)
68	1615	(0)	1529	(14)	1531	(14)	1533	(13)
69	1615	(0)	1529	(14)	1531	(14)	1533	(13)
70	1644	(0)	1581	(0)	1584	(0)	1584	(0)
71	1644	(0)	1605	(2)	1607	(2)	1609	(1)
72	1649	(0)	1605	(2)	1607	(2)	1609	(1)
73	3173	(0)	1642	(4)	1640	(2)	1640	(2)
74	3174	(2.1)	1642	(4)	1640	(2)	1640	(2)
75	3174	(2)	1649	(0)	1648	(0)	1647	(0)
76	3188	(31)	3193	(0)	3190	(0)	3188	(0)
77	3188	(31)	3193	(0)	3191	(0)	3189	(0)
78	3190	(0)	3193	(0)	3191	(0)	3189	(0)
79	3208	(0)	3204	(1)	3202	(3)	3200	(4)
80	3210	(0)	3204	(1)	3202	(3)	3200	(4)
81	3210	(0.)	3206	(0)	3204	(0)	3202	(0)
82	3227	(29)	3221	(0)	3216	(0)	3214	(0)
83	3227	(29)	3223	(0)	3219	(0)	3217	(0)
84	3229	(0)	3223	(0)	3219	(0)	3217	(0)
85			3239	(3)	3235	(6)	3233	(8)

86	3239 (3)	3235 (6)	3233 (8)
87	3241 (0)	3236 (0)	3235 (0)

No.	**5**	**5-Li$^+$**	**5-Na$^+$**	**5-K$^+$**
1	151 (3)	152 (9)	84 (11)	63 (7)
2	214 (0)	193 (6)	98 (4)	79 (2)
3	366 (1)	278 (19)	173 (7)	143 (24)
4	387 (0)	291 (6)	207 (28)	175 (1)
5	444 (0)	370 (2)	224 (0)	222 (0)
6	545 (11)	397 (2)	368 (1)	368 (1)
7	579 (0)	407 (78)	393 (0)	392 (0)
8	591 (0)	447 (2)	446 (1)	446 (0)
9	593 (0)	569 (25)	560 (15)	557 (14)
10	752 (6)	586 (0)	586 (0)	585 (0)
11	760 (60)	593 (0)	592 (0)	592 (0)
12	776 (0)	594 (0)	593 (0)	593 (0)
13	806 (0)	748 (8)	748 (6)	749 (6)
14	809 (0)	775 (0)	775 (0)	776 (0)
15	835 (0)	803 (0)	801 (48)	795 (57)
16	872 (1)	808 (10)	802 (0)	802 (0)
17	887 (7)	823 (66)	813 (20)	811 (8)
18	893 (0)	843 (0)	841 (0)	841 (0)
19	946 (3)	876 (2)	875 (1)	875 (1)
20	994 (0)	887 (8)	886 (9)	886 (8)
21	1006 (2)	935 (1)	923 (1)	918 (1)
22	1011 (0)	980 (2)	969 (2)	966 (2)
23	1027 (6)	1001 (10)	1002 (9)	1003 (7)
24	1052 (4)	1012 (0)	1009 (0)	1008 (0)
25	1068 (8)	1019 (4)	1015 (0)	1012 (0)
26	1069 (0)	1025 (0)	1018 (5)	1021 (6)
27	1095 (0)	1059 (3)	1056 (4)	1055 (4)
28	1127 (0)	1060 (12)	1060 (11)	1061 (10)
29	1150 (6)	1065 (0)	1064 (0)	1063 (0)
30	1181 (0)	1099 (0)	1099 (0)	1098 (0)
31	1198 (1)	1126 (0)	1125 (0)	1127 (0)
32	1219 (4)	1166 (4)	1160 (5)	1157 (5)
33	1223 (3)	1186 (0)	1184 (0)	1184 (0)
34	1229 (0)	1199 (1)	1196 (1)	1197 (1)
35	1262 (0)	1218 (3)	1215 (3)	1214 (3)
36	1279 (13)	1220 (10)	1222 (8)	1222 (8)
37	1334 (0)	1235 (0)	1234 (0)	1233 (0)
38	1387 (0)	1269 (2)	1268 (2)	1268 (1)

39	1480	(12)	1283	(17)	1283	(16)	1282	(16)
40	1491	(4)	1336	(1)	1336	(1)	1336	(1)
41	1493	(3)	1376	(3)	1376	(2)	1382	(2)
42	1528	(3)	1470	(22)	1471	(19)	1475	(18)
43	1634	(0)	1478	(9)	1480	(7)	1485	(7)
44	1651	(0)	1500	(8)	1498	(7)	1496	(6)
45	3052	(56)	1534	(3)	1534	(3)	1533	(3)
46	3059	(43)	1604	(2)	1612	(1)	1619	(1)
47	3114	(23)	1618	(0)	1627	(0)	1633	(0)
48	3118	(39)	3039	(51)	3019	(81)	3021	(91)
49	3125	(66)	3085	(12)	3083	(14)	3081	(16)
50	3126	(27)	3135	(9)	3128	(12)	3125	(15)
51	3163	(4)	3151	(6)	3147	(8)	3145	(6)
52	3170	(3)	3156	(16)	3151	(22)	3147	(27)
53	3179	(31)	3156	(6)	3151	(9)	3148	(14)
54	3191	(21)	3187	(0)	3179	(0)	3173	(1)
55			3190	(0)	3183	(0)	3178	(0)
56			3198	(0)	3191	(0)	3186	(3)
57			3207	(1)	3201	(0)	3196	(2)

No.	**6**		**6-Li$^+$**		**6-Na$^+$**		**6-K$^+$**	
1	96	(2)	103	(1)	81	(8)	65	(6)
2	140	(0)	141	(2)	82	(11)	66	(6)
3	217	(0)	197	(7)	107	(2)	98	(0)
4	220	(1)	215	(8)	149	(0)	147	(0)
5	227	(1)	229	(2)	204	(32)	149	(25)
6	394	(0)	288	(7)	225	(1)	226	(1)
7	447	(0)	297	(16)	231	(2)	229	(1)
8	469	(0)	395	(2)	241	(2)	235	(1)
9	477	(2)	416	(63)	395	(0)	396	(0)
10	523	(5)	448	(0)	448	(0)	447	(0)
11	560	(0)	476	(3)	474	(1)	473	(1)
12	583	(0)	484	(0)	480	(1)	481	(1)
13	597	(0)	546	(26)	534	(11)	531	(10)
14	667	(0)	566	(0)	565	(0)	564	(0)
15	687	(3)	587	(0)	586	(0)	586	(0)
16	729	(0)	619	(3)	610	(3)	609	(2)
17	789	(0)	668	(0)	667	(0)	667	(0)
18	807	(3)	700	(3)	698	(2)	695	(2)
19	808	(0)	729	(0)	728	(0)	727	(0)
20	816	(12)	786	(0)	787	(0)	787	(0)
21	847	(1)	810	(0)	810	(0)	809	(0)

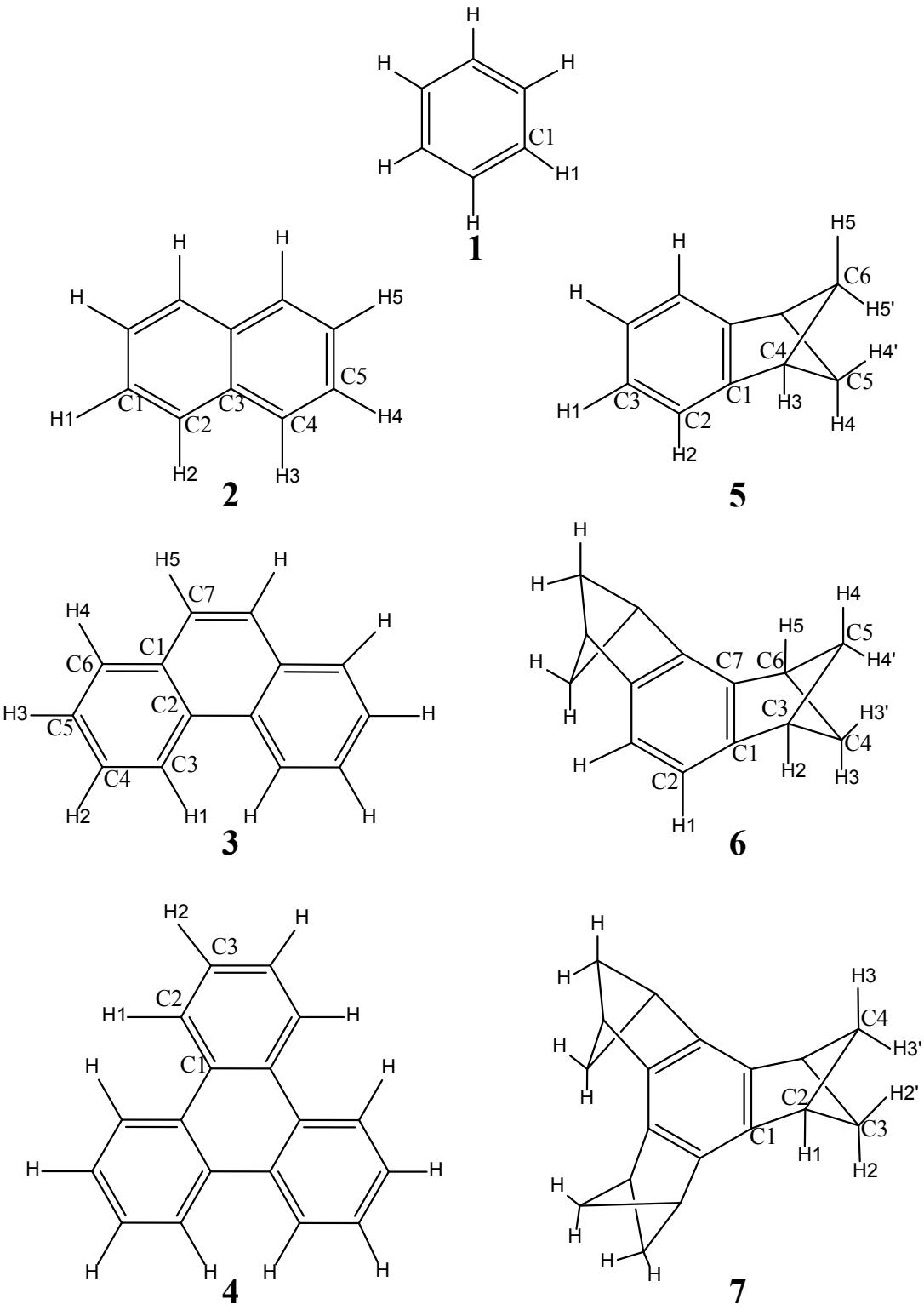
22	848	(0)	811	(0)	810	(0)	809	(0)
23	850	(18)	829	(4)	828	(5)	826	(6)
24	850	(14)	846	(3)	848	(2)	846	(2)
25	872	(9)	848	(11)	848	(14)	848	(20)
26	874	(3)	849	(12)	849	(8)	849	(1)
27	917	(3)	874	(3)	872	(7)	869	(27)
28	939	(0)	874	(9)	874	(8)	872	(8)
29	939	(2)	887	(31)	875	(25)	873	(3)
30	1006	(1)	923	(3)	922	(3)	920	(3)
31	1007	(1)	941	(4)	940	(3)	940	(2)
32	1010	(0)	972	(0)	959	(0)	956	(0)
33	1010	(0)	1002	(2)	1002	(2)	1002	(1)
34	1053	(3)	1006	(1)	1006	(3)	1006	(2)
35	1066	(0)	1007	(6)	1006	(2)	1006	(3)
36	1066	(0)	1011	(0)	1011	(1)	1011	(1)
37	1069	(11)	1046	(3)	1044	(3)	1046	(3)
38	1094	(0)	1064	(16)	1061	(1)	1060	(0)
39	1095	(0)	1064	(3)	1062	(0)	1061	(0)
40	1098	(3)	1065	(0)	1063	(17)	1064	(16)
41	1109	(1)	1095	(2)	1094	(2)	1094	(2)
42	1113	(9)	1097	(0)	1097	(0)	1097	(0)
43	1171	(2)	1102	(2)	1102	(2)	1101	(2)
44	1185	(0)	1105	(1)	1104	(1)	1105	(1)
45	1215	(0)	1125	(9)	1122	(9)	1119	(10)
46	1221	(7)	1180	(0)	1179	(1)	1179	(2)
47	1223	(5)	1188	(1)	1183	(2)	1181	(0)
48	1224	(0)	1215	(0)	1212	(0)	1210	(0)
49	1228	(0)	1220	(10)	1217	(6)	1215	(6)
50	1228	(0)	1221	(0)	1222	(0)	1223	(0)
51	1253	(10)	1221	(11)	1223	(14)	1223	(12)
52	1265	(1)	1233	(0)	1232	(0)	1231	(0)
53	1270	(0)	1234	(1)	1233	(1)	1232	(1)
54	1282	(14)	1255	(12)	1254	(11)	1254	(10)
55	1317	(3)	1271	(2)	1272	(2)	1271	(3)
56	1426	(2)	1273	(4)	1272	(3)	1272	(1)
57	1436	(12)	1289	(15)	1289	(15)	1288	(14)
58	1468	(6)	1325	(5)	1323	(5)	1321	(4)
59	1491	(0)	1409	(2)	1411	(2)	1416	(2)
60	1491	(6)	1422	(15)	1424	(14)	1427	(14)
61	1526	(2)	1450	(11)	1453	(11)	1458	(10)
62	1528	(1)	1499	(0)	1497	(0)	1496	(0)
63	1656	(0)	1500	(16)	1498	(14)	1497	(12)
64	1689	(2)	1535	(3)	1532	(2)	1532	(3)

65	3051	(0)	1537	(1)	1534	(1)	1534	(2)
66	3051	(113)	1619	(2)	1628	(1)	1635	(1)
67	3058	(82)	1649	(2)	1661	(2)	1667	(2)
68	3058	(20)	3037	(0)	3013	(0)	3017	(0)
69	3113	(0)	3038	(103)	3015	(164)	3018	(186)
70	3113	(46)	3083	(4)	3080	(6)	3078	(8)
71	3116	(67)	3083	(25)	3080	(28)	3078	(28)
72	3117	(20)	3131	(12)	3125	(17)	3121	(21)
73	3124	(18)	3131	(10)	3125	(11)	3121	(14)
74	3125	(44)	3148	(9)	3144	(11)	3142	(9)
75	3125	(64)	3148	(9)	3144	(10)	3142	(13)
76	3128	(62)	3154	(23)	3149	(31)	3145	(41)
77	3165	(9)	3154	(8)	3149	(10)	3145	(10)
78	3180	(26)	3155	(0)	3150	(1)	3147	(2)
79			3158	(22)	3153	(28)	3150	(33)
80			3187	(0)	3178	(1)	3172	(2)
81			3197	(0)	3190	(1)	3184	(4)

No.	**7**		**7-Li$^+$**		**7-Na$^+$**		**7-K$^+$**	
1	81	(3)	88	(0)	82	(0)	65	(6)
2	117	(0)	118	(1)	83	(10)	65	(6)
3	118	(0)	118	(1)	90	(9)	81	(1)
4	201	(0)	199	(0)	122	(0)	120	(0)
5	214	(1)	207	(2)	123	(1)	121	(0)
6	215	(1)	208	(2)	199	(0)	151	(26)
7	229	(0)	231	(8)	210	(32)	199	(0)
8	230	(0)	232	(8)	217	(1)	216	(1)
9	374	(0)	295	(7)	217	(1)	217	(1)
10	420	(0)	300	(7)	238	(2)	240	(2)
11	421	(0)	375	(0)	240	(2)	241	(2)
12	515	(2)	412	(59)	376	(0)	377	(0)
13	555	(0)	422	(0)	420	(0)	421	(0)
14	556	(0)	422	(0)	421	(0)	421	(0)
15	575	(0)	541	(28)	525	(8)	521	(7)
16	577	(0)	561	(1)	561	(1)	560	(1)
17	578	(0)	563	(1)	562	(1)	562	(1)
18	598	(0)	573	(0)	573	(0)	572	(0)
19	693	(0)	598	(1)	588	(1)	587	(2)
20	695	(0)	598	(1)	589	(1)	587	(2)
21	705	(0)	602	(0)	603	(1)	603	(1)
22	793	(0)	704	(1)	701	(1)	699	(1)
23	795	(3)	706	(1)	702	(1)	701	(1)

24	797	(3)	707	(0)	706	(0)	705	(0)
25	807	(0)	789	(0)	789	(0)	791	(0)
26	808	(0)	796	(3)	795	(3)	794	(3)
27	809	(0)	796	(3)	795	(3)	794	(3)
28	830	(0)	812	(0)	811	(0)	811	(0)
29	831	(0)	812	(0)	811	(0)	811	(0)
30	853	(0)	813	(0)	811	(0)	811	(0)
31	861	(0)	837	(1)	835	(1)	834	(1)
32	863	(21)	837	(1)	835	(1)	835	(1)
33	864	(21)	849	(0)	847	(0)	850	(0)
34	891	(0)	859	(0)	856	(1)	858	(1)
35	898	(0)	863	(25)	863	(23)	863	(22)
36	899	(0)	864	(25)	863	(23)	863	(22)
37	982	(3)	895	(0)	895	(0)	895	(0)
38	982	(3)	905	(0)	903	(0)	902	(0)
39	1005	(0)	905	(0)	904	(0)	903	(0)
40	1005	(3)	983	(9)	983	(7)	983	(6)
41	1009	(0)	983	(9)	984	(7)	984	(6)
42	1009	(0)	1002	(1)	1000	(1)	998	(2)
43	1038	(1)	1007	(1)	1005	(0)	1003	(0)
44	1040	(4)	1007	(0)	1005	(0)	1003	(0)
45	1040	(4)	1007	(0)	1006	(11)	1006	(1)
46	1065	(0)	1031	(1)	1028	(0)	1030	(0)
47	1065	(0)	1038	(2)	1037	(2)	1037	(2)
48	1066	(0)	1039	(2)	1038	(2)	1037	(2)
49	1074	(5)	1064	(0)	1060	(0)	1059	(0)
50	1075	(5)	1065	(0)	1061	(0)	1060	(1)
51	1092	(0)	1065	(0)	1061	(0)	1060	(0)
52	1092	(0)	1069	(13)	1067	(11)	1068	(10)
53	1092	(0)	1069	(13)	1068	(11)	1068	(10)
54	1108	(0)	1096	(0)	1095	(0)	1095	(0)
55	1113	(9)	1097	(0)	1096	(0)	1096	(0)
56	1114	(9)	1097	(0)	1096	(0)	1097	(0)
57	1174	(0)	1110	(0)	1109	(0)	1109	(0)
58	1187	(0)	1126	(10)	1122	(10)	1120	(10)
59	1221	(4)	1126	(10)	1123	(10)	1121	(10)
60	1222	(5)	1166	(0)	1165	(0)	1166	(0)
61	1222	(0)	1204	(0)	1198	(0)	1195	(0)
62	1222	(5)	1222	(1)	1217	(4)	1216	(4)
63	1223	(1)	1222	(4)	1218	(4)	1216	(4)
64	1226	(0)	1222	(11)	1223	(1)	1223	(0)
65	1226	(0)	1223	(8)	1224	(15)	1224	(4)
66	1227	(0)	1223	(3)	1224	(0)	1224	(9)

67	1231	(0)	1229	(0)	1225	(0)	1225	(0)
68	1266	(0)	1234	(1)	1232	(1)	1232	(1)
69	1266	(0)	1234	(1)	1233	(1)	1232	(1)
70	1274	(0)	1236	(0)	1235	(0)	1235	(0)
71	1284	(15)	1265	(4)	1265	(3)	1266	(2)
72	1285	(15)	1266	(4)	1265	(3)	1266	(2)
73	1327	(0)	1285	(0)	1283	(0)	1281	(0)
74	1368	(10)	1292	(19)	1291	(18)	1290	(18)
75	1369	(10)	1292	(20)	1291	(18)	1290	(18)
76	1490	(0)	1340	(0)	1336	(0)	1333	(0)
77	1490	(0)	1353	(8)	1353	(8)	1357	(8)
78	1491	(10)	1353	(7)	1353	(7)	1358	(8)
79	1518	(0)	1498	(0)	1496	(0)	1494	(0)
80	1524	(2)	1498	(12)	1496	(6)	1495	(1)
81	1525	(2)	1498	(13)	1497	(18)	1495	(18)
82	1551	(0)	1506	(0)	1510	(0)	1514	(0)
83	1710	(2)	1532	(2)	1530	(2)	1528	(2)
84	1710	(2)	1533	(2)	1531	(2)	1530	(2)
85	3049	(19)	1542	(0)	1542	(1)	1543	(2)
86	3049	(0)	1666	(3)	1679	(3)	1686	(3)
87	3050	(150)	1666	(3)	1679	(3)	1686	(3)
88	3056	(85)	3035	(4)	3012	(0)	3014	(1)
89	3057	(86)	3035	(0)	3012	(2)	3014	(0)
90	3058	(0)	3036	(151)	3014	(243)	3016	(277)
91	3111	(1)	3080	(6)	3078	(8)	3076	(10)
92	3111	(0)	3080	(5)	3079	(7)	3076	(9)
93	3112	(68)	3080	(39)	3079	(41)	3077	(41)
94	3115	(71)	3128	(14)	3122	(19)	3118	(23)
95	3115	(73)	3128	(12)	3122	(14)	3118	(18)
96	3116	(1)	3129	(13)	3123	(14)	3119	(17)
97	3125	(1)	3144	(15)	3142	(15)	3139	(16)
98	3126	(1)	3144	(15)	3142	(16)	3139	(17)
99	3126	(0)	3144	(8)	3142	(8)	3140	(9)
100	3129	(138)	3152	(0)	3146	(0)	3143	(0)
101	3129	(137)	3153	(0)	3147	(0)	3143	(0)
102	3131	(1)	3153	(0)	3147	(1)	3143	(1)
103			3155	(39)	3149	(55)	3146	(66)
104			3155	(43)	3150	(57)	3146	(66)
105			3156	(5)	3150	(2)	3147	(1)



Scheme S1: Structures of ligands with atom numbering that was used for providing NMR chemical shift values.

Table S4: ^{13}C and ^{1}H NMR chemical shift values for ligands obtained at the B3LYP/6-311+G(2d,2p) and B3LYP/6-31++G(3df,2p) levels along with the experimental values. Computed chemical shift values are in reference to tetramethylsilane (TMS).

	B3LYP/ 6-311+G(2d,2p)	B3LYP/ 6-31++G(3df,2p)	Experimental
Ligand (**1**)[a,b]			
C1	134.94	125.73	128.36
H1	7.78	7.72	7.34
Ligand (**2**)[b]			
C1	132.14	122.96	125.75
C2	134.93	125.42	127.84
C3	142.33	134.21	133.45
C4	134.93	125.42	127.84
C5	132.14	122.96	125.75
H1	7.91	7.85	7.48
H2	8.36	8.36	7.84
H3	8.36	8.36	7.84
H4	7.91	7.85	7.48
Ligand (**3**)[b]			
C1	140.81	133.61	131.99
C2	139.01	131.90	130.25
C3	128.90	121.35	122.59
C4	132.45	123.26	-
C5	132.80	123.86	126.46
C6	135.00	126.35	128.46
C7	134.33	126.40	126.84
H1	9.27	9.25	8.65
H2	8.10	8.04	7.61
H3	8.04	7.98	7.57
H4	8.31	8.34	7.86
H5	8.20	8.15	7.70
Ligand (**4**)[b]			
C1	138.65	132.09	129.82
C2	128.84	120.68	123.31
C3	132.74	124.78	127.21

H1	9.27	9.24	8.64
H2	8.04	7.95	7.64
Ligand (**7**)[c]			
C1	144.35	136.42	135.89
C2	50.44	49.81	43.96
C3	64.32	62.83	58.66
C4	64.32	62.83	58.66
H1	3.25	3.35	3.22
H2	2.27	2.11	2.27
H2′	2.86	2.81	2.52
H3	2.27	2.11	2.27
H3′	2.86	2.81	2.52

[a]Experimental values were taken from ref. Pouchert, C. J.; Behnke, J. *The Aldrich Library of* ^{13}C *and* ^{1}H *FT NMR Spectra*, 1st ed.; Aldrich: St. Louis, MO, 1993.

[b]Experimental values were taken from ref. National Institute of Advanced Industrial Science and Technology (AIST), Japan. Spectral Database for Organic Compounds, SDBS. http://riodb01.ibase.aist.go.jp/sdbs/.

[c]Experimental values were taken from ref. Frank, N. L.; Baldridge, K. K.; Siegel, J. S. *J. Am. Chem. Soc.* **1995**, *117*, 2102.

Table S5: ^{13}C and ^{1}H NMR chemical shift values obtained for ligands and complexes at the B3LYP/6-31++G(3df,2p) level. The computed chemical shift values are in reference to tetramethylsilane (TMS).

System 1				
	Ligand (**1**)	**1-Li$^+$**	**1-Na$^+$**	**1-K$^+$**
C1	125.73	129.55	128.68	128.45
H1	7.72	8.50	8.42	8.26

System 2				
	Ligand (**2**)	**2-Li$^+$**	**2-Na$^+$**	**2-K$^+$**
C1	122.96	122.29	122.76	123.83
C2	125.42	128.04	127.47	127.96
C3	134.21	130.87	131.11	131.64
C4	125.42	127.29	126.94	126.89
C5	122.96	133.1	130.92	129.45
H1	7.85	8.36	8.33	8.22
H2	8.36	8.86	8.8	8.62
H3	8.36	8.78	8.71	8.56
H4	7.85	8.72	8.60	8.49

System 3				
	Ligand (**3**)	**3-Li$^+$**	**3-Na$^+$**	**3-K$^+$**
C1	133.61	126.81	128.52	129.59
C2	131.90	127.18	127.75	129.28
C3	121.35	123.45	122.4	121.16
C4	123.26	132.31	130.35	129.27
C5	123.86	131.43	129.68	128.19
C6	126.35	128.81	128.09	128.25
C7	126.40	124.35	125.10	125.31
H1	9.25	9.52	9.50	9.47
H2	8.04	8.77	8.67	8.55
H3	7.98	8.68	8.59	8.51
H4	8.34	8.77	8.70	8.59
H5	8.15	8.60	8.53	8.42

System 4				
	Ligand (**4**)	**4-Li$^+$**	**4-Na$^+$**	**4-K$^+$**
C1	132.09	125.17	126.74	128.69

C2	120.68	123.71	122.92	122.15
C3	124.78	131.37	130.01	128.90
H1	9.24	9.51	9.46	9.41
H2	7.95	8.67	8.57	8.48

System 5

	Ligand (**5**)	**5-Li$^+$**	**5-Na$^+$**	**5-K$^+$**
C1	151.05	160.68	158.86	157.55
C2	116.94	120.53	119.38	119.55
C3	121.29	122.76	122.57	122.88
C4	50.35	52.52	52.02	51.9
C5	66.19	70.91	71.29	68.66
C6	66.19	69.65	68.14	68.51
H1	7.33	7.94	7.86	7.73
H2	7.54	8.14	8.11	7.96
H3	3.17	3.68	3.64	3.56
H4	2.43	2.23	2.0	1.96
H4′	2.88	3.46	3.5	3.42
H5	2.43	2.94	2.88	2.84
H5′	2.88	3.36	3.31	3.28

System 6

	Ligand (**6**)	**6-Li$^+$**	**6-Na$^+$**	**6-K$^+$**
C1	147.19	154.79	152.96	152.01
C2	113.92	113.55	112.86	111.87
C3	53.71	53.73	53.18	53.61
C4	65.72	69.09	68.30	66.42
C5	65.72	68.06	66.02	67.37
C6	50.02	51.03	51.50	49.64
C7	141.29	148.8	146.8	145.59
H1	7.08	7.6	7.61	7.43
H2	3.22	3.67	3.58	3.54
H3	2.26	1.98	1.82	1.68
H3′	3.22	3.67	3.58	3.54
H4	2.26	2.66	2.63	2.57
H4′	2.87	3.28	3.16	3.15
H5	3.20	3.66	3.67	3.61

System 7

	Ligand (**7**)	**7-Li$^+$**	**7-Na$^+$**	**7-K$^+$**

C1	136.42	142.36	140.82	140.19
C2	49.81	50.40	52.55	51.85
C3	62.83	65.87	67.80	64.10
C4	62.83	63.9	65.07	66.09
H1	3.35	3.72	3.72	3.63
H2	2.11	1.81	1.52	1.50
H2′	2.81	3.29	3.45	3.32
H3	2.11	2.51	2.46	2.39
H3′	2.81	3.16	3.23	3.17

Table S6: Atomic Contributions to the Total Energy, E(Ω), of phenanthrene and triphenylene and their corresponding linear counterparts anthracene and naphthacene (in hartree) calculated with the Quantum Theory of Atoms in Molecules (QTAIM) at the B3LYP/6-311+G(2d,2p) level. (See Scheme 2 for atom numbering)

Phenanthrene		Anthracene		Triphenylene		Naphthacene	
E(Ω), hartree		E(Ω), hartree		E(Ω), hartree		E(Ω), hartree	
C1	-38.09758	C1	-38.09358	C1	-38.10024	C1	-38.09297
C2	-38.09392	C2	-38.08860	C2	-38.09756	C2	-38.08777
C3	-38.09144	C3	-38.08860	C3	-38.09756	C3	-38.08777
C4	-38.09485	C4	-38.09358	C4	-38.10024	C4	-38.09297
C5	-38.09485	C5	-38.09358	C5	-38.10024	C5	-38.09732
C6	-38.09144	C6	-38.08860	C6	-38.09756	C6	-38.09732
C7	-38.09392	C7	-38.08860	C7	-38.09756	C7	-38.09297
C8	-38.09758	C8	-38.09358	C8	-38.10024	C8	-38.08777
C9	-38.10034	C9	-38.09846	C9	-38.10024	C9	-38.08777
C10	-38.10034	C10	-38.09846	C10	-38.09756	C10	-38.09297
C11	-38.12279	C11	-38.12279	C11	-38.09756	C11	-38.09732
C12	-38.10143	C12	-38.12279	C12	-38.10024	C12	-38.09732
C13	-38.10143	C13	-38.12279	C13	-38.09946	C13	-38.12114
C14	-38.12279	C14	-38.12279	C14	-38.09946	C14	-38.12114
H15	-0.62739	H15	-0.62627	C15	-38.09946	C15	-38.12164
H16	-0.62625	H16	-0.62654	C16	-38.09946	C16	-38.12164
H17	-0.62708	H17	-0.62654	C17	-38.09946	C17	-38.12114
H18	-0.63474	H18	-0.62627	C18	-38.09946	C18	-38.12114
H19	-0.63474	H19	-0.62627	H19	-0.63780	H19	-0.62610
H20	-0.62708	H20	-0.62654	H20	-0.62678	H20	-0.62643
H21	-0.62625	H21	-0.62654	H21	-0.62678	H21	-0.62643
H22	-0.62739	H22	-0.62627	H22	-0.63780	H22	-0.62610
H23	-0.62675	H23	-0.62651	H23	-0.63780	H23	-0.62638
H24	-0.62675	H24	-0.62651	H24	-0.62678	H24	-0.62638
				H25	-0.62678	H25	-0.62610
				H26	-0.63780	H26	-0.62643
				H27	-0.63780	H27	-0.62643
				H28	-0.62678	H28	-0.62610
				H29	-0.62678	H29	-0.62638
				H30	-0.63780	H30	-0.62638

Table S7: Atomic energy (in hartrees), E(Ω) obtained with atomic integration of atomic basins by QTAIM at the B3LYP/6-311+G(2d,2p) level. The table lists the sum of atomic energy of all carbon atoms, $\sum E(\Omega_C)$; sum of atomic energy of all hydrogen atoms, $\sum E(\Omega_H)$; average energy of all hydrogen atoms, $\overline{E}_H$; and average energy of hydrogen atoms involved in hydrogen-hydrogen interaction, $\overline{E}_{H\cdots H}$; all these values are reported in hartrees. The following entities $\Delta E(\Omega_C)$, $\Delta E(\Omega_H)$, $[\Delta E(\Omega_H)+\Delta E(\Omega_C)]$, $\Delta \overline{E}_H$, $(\overline{E}_{H\cdots H} - \overline{E}_H)$ are reported in kcal/mol. (See Table S6 for individual atomic contributions to total energies of systems).

	Case I		Case II	
	Phenanthrene	Anthracene	Triphenylene	Naphthacene
Sum of atomic energy of all carbon atoms, $\sum E(\Omega_C)$	–533.40470	–533.41681	–685.78352	–685.8401
$\Delta E(\Omega_C)$,[a] kcal/mol	+7.60	0.0	+35.50	0.0
Sum of atomic energy of all hydrogen atoms, $\sum E(\Omega_H)$	–6.28444	–6.26426	–7.58751	–7.51562
$\Delta E(\Omega_H)$,[a,b] kcal/mol	–12.66	0.0	–45.11	0.0
$[\Delta E(\Omega_H)+\Delta E(\Omega_C)]$,[c] kcal/mol	–5.06	0.0	–9.61	0.0
Average energy of hydrogen atoms, $\overline{E}_H$	–0.62687 [d]	–0.62643	–0.62678 [d]	–0.62630
$\Delta \overline{E}_H$, kcal/mol	–0.28	0.0	–0.30	0.0
Average energy of the hydrogen atoms involved in H···H interaction, $\overline{E}_{HH}$	–0.63474	NA [e]	–0.63780	NA [e]
$(\overline{E}_{H\ldots H} - \overline{E}_H)$, kcal/mol	–5.22 [f]	NA [e]	–7.22 [f]	NA [e]

[a] Calculated as nonlinear – linear aromatic system; for example, Phenanthrene – Anthracene.
[b] The negative values indicate the hydrogen atoms of nonlinear aromatic compound is more stabilized compared to linear aromatic system.
[c] The negative values indicate nonlinear aromatic compound is more stabilized compared to linear aromatic system. Phenanthrene is more stable by 5.06 kcal/mol than anthracene; triphenylene is more stable by 9.61 kcal/mol than naphthacene.
[d] Average energy of all hydrogen atoms not involved in hydrogen-hydrogen interaction in the cyclic system
[e] NA means not applicable.
[f] Difference in energy between the average energy of the hydrogen involved in H···H interaction in the cyclic system and the average energy of all hydrogen atoms in the linear counterpart.

Table S8: Selected vibrational frequencies (ν_{C-H}, in cm^{-1}) corresponding to C–H bonds of bridge CH_2 unit (that is not on the side of metal ion binding) of bicyclo[2.1.1]hexenyl moiety of ligands (**5**-**7**) and their complexes obtained at the B3LYP/6-311+G(2d,2p) level. Intensities (km/mol) are given in parentheses.

	Endo C–H bond length	ν_{C-H}, in cm^{-1} [(a)]	Exo C–H bond length	ν_{C-H}, in cm^{-1} [(b)]
5	1.088	3052 (57)	1.090	3114 (23)
5Li$^+$	1.087	3085 (12)	1.087	3151 (6)
5Na$^+$	1.087	3083 (14)	1.087	3147 (8)
5K$^+$	1.087	3080 (16)	1.087	3154 (6)
6	1.089	3051 (113)	1.090	3113 (46)
6Li$^+$	1.087	3083(25)	1.087	3148 (9)
6Na$^+$	1.087	3080 (28)	1.087	3144 (11)
6K$^+$	1.087	3078 (29)	1.088	3142 (13)
7	1.089	3050 (150)	1.090	3112 (68)
7Li$^+$	1.087	3080 (39)	1.087	3144 (15)
7Na$^+$	1.087	3079 (41)	1.087	3142 (16)
7K$^+$	1.087	3076 (41)	1.088	3139 (17)

(a) Endo C–H bond experiences more stretching than the exo C–H bond, and the stretching is symmetric.

(b) Exo C–H bond experience more stretching than the endo C–H bond, and the stretching is asymmetric.