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

Electronic Supplementary Information

Ground and excited states analysis of alkali metal ethylenediamine and crown ether complexes

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Table S1. MP2 optimized geometries (Cartesian coordinates in Å) for $M(en)_2$ (M = Li, Na, K).

$Li(en)_2$				$Na(en)_2$				$K(en)_2$			
Li	0.000000	0.000000	0.000000	Na	0.000000	0.000000	0.000000	K	0.000000	0.000000	0.000000
N	1.522049	0.979754	1.026989	N	2.035803	0.997381	1.077960	N	2.641318	1.359931	-0.612682
N	-1.522049	0.979754	-1.026989	N	-2.035803	0.997381	-1.077960	N	-2.641318	-1.359931	-0.612682
N	1.522049	-0.979754	-1.026989	N	2.035803	-0.997381	-1.077960	N	2.641318	-1.359931	0.612682
N	-1.522049	-0.979754	1.026989	N	-2.035803	-0.997381	1.077960	N	-2.641318	1.359931	0.612682
C	2.746271	0.717790	0.247246	C	3.214612	0.720110	0.241848	C	3.791043	0.445632	-0.614275
C	2.746271	-0.717790	-0.247246	C	3.214612	-0.720110	-0.241848	C	3.791043	-0.445632	0.614275
C	-2.746271	-0.717790	0.247246	C	-3.214612	-0.720110	0.241848	C	-3.791043	0.445632	0.614275
C	-2.746271	0.717790	-0.247246	C	-3.214612	0.720110	-0.241848	C	-3.791043	-0.445632	-0.614275
H	1.617568	-0.578909	-1.956966	H	2.153229	-0.561085	-1.988570	H	2.772711	-2.067301	-0.103345
H	1.406700	-1.979572	-1.172947	H	1.964886	-1.994609	-1.260758	H	2.599898	-1.865850	1.490996
H	1.617568	0.578909	1.956966	H	2.153229	0.561085	1.988570	H	2.772711	2.067301	0.103345
H	1.406700	1.979572	1.172947	H	1.964886	1.994609	1.260758	H	2.599898	1.865850	-1.490996
H	-1.617568	-0.578909	1.956966	H	-2.153229	-0.561085	1.988570	H	-2.772711	2.067301	-0.103345
H	-1.406700	-1.979572	1.172947	H	-1.964886	-1.994609	1.260758	H	-2.599898	1.865850	1.490996
H	-1.406700	1.979572	-1.172947	H	-1.964886	1.994609	-1.260758	H	-2.599898	-1.865850	-1.490996
H	-1.617568	0.578909	-1.956966	H	-2.153229	0.561085	-1.988570	H	-2.772711	-2.067301	0.103345
H	3.660386	0.907534	0.815964	H	4.157587	0.914800	0.760628	H	4.752175	0.967089	-0.660666
H	3.660386	-0.907534	-0.815964	H	4.157587	-0.914800	-0.760628	H	4.752175	-0.967089	0.660666
H	2.747225	-1.393751	0.607718	H	3.177537	-1.386800	0.620182	H	3.722833	0.179051	1.506130
H	2.747225	1.393751	-0.607718	H	3.177537	1.386800	-0.620182	H	3.722833	-0.179051	-1.506130
H	-2.747225	-1.393751	-0.607718	H	-3.177537	-1.386800	-0.620182	H	-3.722833	-0.179051	1.506130
H	-3.660386	-0.907534	0.815964	H	-4.157587	-0.914800	0.760628	H	-4.752175	0.967089	0.660666
H	-2.747225	1.393751	0.607718	H	-3.177537	1.386800	0.620182	H	-3.722833	0.179051	-1.506130
H	-3.660386	0.907534	-0.815964	H	-4.157587	0.914800	-0.760628	H	-4.752175	-0.967089	-0.660666

Table S2. MP2 optimized geometries (Cartesian coordinates in Å) for M(12C4) (M = Li, Na, K).

Li(12C4)				Na(12C4)				K(12C4)			
O	0.000000	1.997913	0.439899	O	0.000000	1.586063	0.181225	O	0.000000	1.728866	-0.042266
O	-1.565783	0.000000	-0.272763	O	-2.152444	0.000000	-0.796518	O	-1.996526	0.000000	-1.054735
O	1.565783	-0.000000	-0.272763	O	2.152444	-0.000000	-0.796518	O	1.996526	-0.000000	-1.054735
O	-0.000000	-1.997913	0.439899	O	-0.000000	-1.586063	0.181225	O	-0.000000	-1.728866	-0.042266
C	1.210220	2.297931	-0.249624	C	1.184019	2.130406	-0.384724	C	1.188865	2.186697	-0.665987
C	-2.209114	1.214755	0.100389	C	-2.336150	1.206212	-0.079464	C	-2.292140	1.201912	-0.372782
C	2.209114	1.214755	0.100389	C	2.336150	1.206212	-0.079464	C	2.292140	1.201912	-0.372782
C	-2.209114	-1.214755	0.100389	C	-2.336150	-1.206212	-0.079464	C	-2.292140	-1.201912	-0.372782
C	2.209114	-1.214755	0.100389	C	2.336150	-1.206212	-0.079464	C	2.292140	-1.201912	-0.372782
C	-1.210220	-2.297931	-0.249624	C	-1.184019	-2.130406	-0.384724	C	-1.188865	-2.186697	-0.665987
C	1.210220	-2.297931	-0.249624	C	1.184019	-2.130406	-0.384724	C	1.188865	-2.186697	-0.665987
C	-1.210220	2.297931	-0.249624	C	-1.184019	2.130406	-0.384724	C	-1.188865	2.186697	-0.665987
H	1.587940	3.279489	0.043989	H	1.383114	3.128357	0.020431	H	1.463814	3.182421	-0.301920
H	1.031769	2.287034	-1.327584	H	1.069074	2.205570	-1.469612	H	1.044694	2.235447	-1.748996
H	-2.422657	1.214429	1.173735	H	-2.388507	1.020303	0.997451	H	-2.358710	1.033115	0.706273
H	-3.139158	1.357374	-0.457745	H	-3.271937	1.687478	-0.378557	H	-3.250160	1.615100	-0.703834
H	3.139158	1.357374	-0.457745	H	3.271937	1.687478	-0.378557	H	3.250160	1.615100	-0.703834
H	2.422657	1.214429	1.173735	H	2.388507	1.020303	0.997451	H	2.358710	1.033115	0.706273
H	-3.139158	-1.357374	-0.457745	H	-3.271937	-1.687478	-0.378557	H	-3.250160	-1.615100	-0.703834
H	-2.422657	-1.214429	1.173735	H	-2.388507	-1.020303	0.997451	H	-2.358710	-1.033115	0.706273
H	2.422657	-1.214429	1.173735	H	2.388507	-1.020303	0.997451	H	2.358710	-1.033115	0.706273
H	3.139158	-1.357374	-0.457745	H	3.271937	-1.687478	-0.378557	H	3.250160	-1.615100	-0.703834
H	-1.587940	-3.279489	0.043989	H	-1.383114	-3.128357	0.020431	H	-1.463814	-3.182421	-0.301920
H	-1.031769	-2.287034	-1.327584	H	-1.069074	-2.205570	-1.469612	H	-1.044694	-2.235447	-1.748996
H	1.031769	-2.287034	-1.327584	H	1.069074	-2.205570	-1.469612	H	1.044694	-2.235447	-1.748996
H	1.587940	-3.279489	0.043989	H	1.383114	-3.128357	0.020431	H	1.463814	-3.182421	-0.301920
H	-1.587940	3.279489	0.043989	H	-1.383114	3.128357	0.020431	H	-1.463814	3.182421	-0.301920
H	-1.031769	2.287034	-1.327584	H	-1.069074	2.205570	-1.469612	H	-1.044694	2.235447	-1.748996
Li	0.000000	0.000000	1.059294	Na	0.000000	0.000000	2.209668	K	0.000000	0.000000	2.667177

Table S3. MP2 optimized geometries (Cartesian coordinates in Å) for M(15C5) (M = Li, Na, K).

Li(15C5)				Na(15C5)				K(15C5)			
O	2.127232	0.700992	-0.240642	O	0.001394	-2.009339	-0.403170	O	-0.014057	-1.969988	-0.565176
O	1.285257	-1.734291	0.130862	O	-2.311861	-0.756453	0.309156	O	-2.406580	-0.756362	0.123804
O	0.001234	2.068350	0.000021	O	2.325318	-0.787753	0.564277	O	2.405973	-0.813556	0.381205
O	-1.287563	-1.732995	-0.131258	O	-1.348284	1.693365	-0.343261	O	-1.328969	1.689036	-0.504624
O	-2.126387	0.703517	0.240813	O	1.375359	1.807353	0.116754	O	1.437576	1.838452	-0.035908
C	0.695469	-2.963115	-0.279873	C	-3.182705	0.240791	-0.202651	C	-3.203199	0.277909	-0.429172
C	1.191858	2.844292	-0.075812	C	2.339116	-1.741615	-0.488152	C	2.330470	-1.755937	-0.677519
C	-0.699045	-2.962277	0.279849	C	-2.647284	1.584284	0.221322	C	-2.642841	1.604914	0.014348
C	3.095131	-0.258115	0.167052	C	-1.140456	-2.779674	-0.045987	C	-1.165768	-2.743737	-0.268735
C	2.614618	-1.583791	-0.352006	C	-2.355571	-1.970774	-0.418702	C	-2.371846	-1.931964	-0.662320
C	-1.188515	2.845685	0.075735	C	3.195286	0.319019	0.354102	C	3.243186	0.297977	0.092833
C	-2.616494	-1.580657	0.352188	C	-0.704181	2.923322	-0.052510	C	-0.679485	2.909842	-0.206449
C	-2.312117	1.958058	-0.395030	C	2.567364	1.380994	-0.521060	C	2.557088	1.349561	-0.748937
C	-3.095452	-0.254421	-0.166835	C	0.690223	2.816862	-0.612146	C	0.713774	2.813719	-0.769150
C	2.314513	1.955432	0.394942	C	1.221001	-2.715987	-0.225805	C	1.190314	-2.696035	-0.393708
H	3.283678	2.389300	0.128897	H	1.280745	-3.554713	-0.927425	H	1.230195	-3.542305	-1.090575
H	1.264871	-3.811622	0.109767	H	-4.200226	0.099676	0.173700	H	-4.245161	0.181678	-0.107957
H	0.674215	-3.015062	-1.371662	H	-3.197084	0.190930	-1.295700	H	-3.163514	0.231851	-1.521987
H	1.122084	3.722988	0.570912	H	3.300307	-2.264953	-0.506968	H	3.269334	-2.316948	-0.747093
H	1.344392	3.166489	-1.108453	H	2.176059	-1.262232	-1.457751	H	2.141248	-1.260731	-1.634574
H	-1.269329	-3.810349	-0.109448	H	-3.303014	2.378346	-0.152584	H	-3.271971	2.413531	-0.375656
H	-0.677767	-3.013889	1.371659	H	-2.595657	1.652932	1.312987	H	-2.636134	1.676967	1.107988
H	3.155429	-0.280034	1.258805	H	-1.131505	-2.990948	1.027959	H	-1.198322	-2.995515	0.797021
H	4.079444	-0.012780	-0.242602	H	-1.151393	-3.727962	-0.593886	H	-1.161678	-3.677788	-0.841969
H	2.615369	-1.597877	-1.445244	H	-2.331715	-1.758334	-1.492237	H	-2.283251	-1.666460	-1.721326
H	3.251356	-2.392430	0.017859	H	-3.264776	-2.535767	-0.188847	H	-3.280361	-2.529160	-0.520905
H	-1.117671	3.724248	-0.571045	H	4.143339	-0.011999	-0.080667	H	4.159848	-0.029289	-0.408933
H	-1.340716	3.168122	1.108347	H	3.385326	0.735390	1.341736	H	3.512380	0.729301	1.056151
H	-2.616779	-1.594547	1.445434	H	-0.666065	3.092036	1.028690	H	-0.642810	3.081080	0.875462
H	-3.254477	-2.388508	-0.017235	H	-1.232833	3.759354	-0.523364	H	-1.204057	3.753605	-0.669592
H	-3.280811	2.393113	-0.129241	H	3.269033	2.215532	-0.632733	H	3.273282	2.155331	-0.953869
H	-2.266681	1.827569	-1.480424	H	2.334395	0.994781	-1.519718	H	2.229160	0.935399	-1.709439
H	-3.155836	-0.276294	-1.258583	H	0.634124	2.539337	-1.669723	H	0.644309	2.515130	-1.820617
H	-4.079452	-0.007909	0.242849	H	1.214044	3.773348	-0.521522	H	1.215182	3.785474	-0.709474
H	2.269113	1.825175	1.480367	H	1.296847	-3.099688	0.796297	H	1.271731	-3.083480	0.628647
Li	0.000529	-0.022280	-0.000200	Na	-0.017466	-0.013252	1.443750	K	-0.023216	-0.053465	2.077218

Table S4. MP2 optimized geometries (Cartesian coordinates in Å) for M(18C6) (M = Na, K).

Na(18C6)				K(18C6)			
H	3.272757	3.231538	-0.039937	H	1.224135	4.484185	-0.255390
O	2.378722	1.373356	0.102067	O	0.000000	2.847985	0.073059
O	0.000000	2.771608	-0.259424	O	2.394820	1.382650	-0.359252
O	2.400283	-1.385804	-0.259424	O	-2.394820	1.382650	-0.359252
O	-2.378722	1.373356	0.102067	O	2.466427	-1.423992	0.073059
O	-0.000000	-2.746711	0.102067	O	-2.466427	-1.423992	0.073059
O	-2.400283	-1.385804	-0.259424	O	-0.000000	-2.765299	-0.359252
C	3.528927	0.687819	-0.353743	C	-1.173210	3.412351	-0.483414
C	-1.166931	3.395428	0.248468	C	3.545945	0.693993	0.103896
C	2.357062	-2.708306	0.248468	C	-3.545945	0.693993	0.103896
C	-2.360132	2.712231	-0.353743	C	3.541788	-0.690146	-0.483414
C	1.168795	-3.400049	-0.353743	C	-3.541788	-0.690146	-0.483414
C	1.166931	3.395428	0.248468	C	2.373988	2.723882	0.103896
C	3.523993	-0.687123	0.248468	C	-2.373988	2.723882	0.103896
C	-3.528927	0.687819	-0.353743	C	2.368577	-2.722205	-0.483414
C	-1.168795	-3.400049	-0.353743	C	-2.368577	-2.722205	-0.483414
C	-3.523993	-0.687123	0.248468	C	1.171957	-3.417875	0.103896
C	-2.357062	-2.708306	0.248468	C	-1.171957	-3.417875	0.103896
C	2.360132	2.712231	-0.353743	C	1.173210	3.412351	-0.483414
H	3.522433	0.620918	-1.447233	H	-1.173900	3.282552	-1.571833
H	4.434972	1.218522	-0.039937	H	-1.224135	4.484185	-0.255390
H	-1.198425	3.306864	1.339039	H	3.547678	0.638568	1.197772
H	-1.177031	4.457457	-0.023103	H	4.454256	1.216432	-0.218784
H	3.271756	-3.248067	-0.023103	H	-4.454256	1.216432	-0.218784
H	2.264616	-2.691299	1.339039	H	-3.547678	0.638568	1.197772
H	-2.298947	2.740057	-1.447233	H	3.429723	-0.624649	-1.571833
H	-3.272757	3.231538	-0.039937	H	4.495485	-1.181961	-0.255390
H	1.162215	-4.450059	-0.039937	H	-4.495485	-1.181961	-0.255390
H	1.223485	-3.360975	-1.447233	H	-3.429723	-0.624649	-1.571833
H	1.177031	4.457457	-0.023103	H	3.280589	3.249283	-0.218784
H	1.198425	3.306864	1.339039	H	2.326856	2.753095	1.197772
H	3.463041	-0.615566	1.339039	H	-2.326856	2.753095	1.197772
H	4.448786	-1.209390	-0.023103	H	-3.280589	3.249283	-0.218784
H	-4.434972	1.218522	-0.039937	H	3.271351	-3.302224	-0.255390
H	-3.522433	0.620918	-1.447233	H	2.255824	-2.657903	-1.571833
H	-1.223485	-3.360975	-1.447233	H	-2.255824	-2.657903	-1.571833
H	-1.162215	-4.450059	-0.039937	H	-3.271351	-3.302224	-0.255390
H	-4.448786	-1.209390	-0.023103	H	1.173667	-4.465715	-0.218784
H	-3.463041	-0.615566	1.339039	H	1.220823	-3.391664	1.197772
H	-3.271756	-3.248067	-0.023103	H	-1.173667	-4.465715	-0.218784
H	-2.264616	-2.691299	1.339039	H	-1.220823	-3.391664	1.197772
H	2.298947	2.740057	-1.447233	H	1.173900	3.282552	-1.571833
Na	0.000000	0.000000	0.781258	K	0.000000	0.000000	1.348457

Table S5. B3LYP optimized geometries (Cartesian coordinates in Å) for $M(en)_2$ (M = Li, Na, K).

$Li(en)_2$				$Na(en)_2$				$K(en)_2$			
Li	0.000000	0.000000	0.000000	Na	0.000000	0.000000	0.000000	K	0.000000	0.000000	0.000000
N	1.506043	0.999597	1.026116	N	1.967008	1.025863	1.077560	N	2.487401	0.989236	1.133371
N	-1.506043	0.999597	-1.026116	N	-1.967008	1.025863	-1.077560	N	-2.487401	0.989236	-1.133371
N	1.506043	-0.999597	-1.026116	N	1.967008	-1.025863	-1.077560	N	2.487401	-0.989236	-1.133371
N	-1.506043	-0.999597	1.026116	N	-1.967008	-1.025863	1.077560	N	-2.487401	-0.989236	1.133371
C	2.738171	0.717105	0.257741	C	3.148879	0.721767	0.246986	C	3.645183	0.714848	0.265803
C	2.738171	-0.717105	-0.257741	C	3.148879	-0.721767	-0.246986	C	3.645183	-0.714848	-0.265803
C	-2.738171	-0.717105	0.257741	C	-3.148879	-0.721767	0.246986	C	-3.645183	-0.714848	0.265803
C	-2.738171	0.717105	-0.257741	C	-3.148879	0.721767	-0.246986	C	-3.645183	0.714848	-0.265803
H	1.585634	-0.623675	-1.968708	H	2.075369	-0.621588	-2.004737	H	2.597362	-0.518232	-2.027229
H	1.378690	-2.003494	-1.137652	H	1.883662	-2.029879	-1.220145	H	2.429244	-1.981398	-1.344069
H	1.585634	0.623675	1.968708	H	2.075369	0.621588	2.004737	H	2.597362	0.518232	2.027229
H	1.378690	2.003494	1.137652	H	1.883662	2.029879	1.220145	H	2.429244	1.981398	1.344069
H	-1.585634	-0.623675	1.968708	H	-2.075369	-0.621588	2.004737	H	-2.597362	-0.518232	2.027229
H	-1.378690	-2.003494	1.137652	H	-1.883662	-2.029879	1.220145	H	-2.429244	-1.981398	1.344069
H	-1.378690	2.003494	-1.137652	H	-1.883662	2.029879	-1.220145	H	-2.429244	1.981398	-1.344069
H	-1.585634	0.623675	-1.968708	H	-2.075369	0.621588	-2.004737	H	-2.597362	0.518232	-2.027229
H	3.647019	0.889474	0.844215	H	4.090291	0.903957	0.777616	H	4.602767	0.889207	0.771423
H	3.647019	-0.889474	-0.844215	H	4.090291	-0.903957	-0.777616	H	4.602767	-0.889207	-0.771423
H	2.765897	-1.406572	0.587200	H	3.133964	-1.395761	0.611220	H	3.603473	-1.410074	0.575266
H	2.765897	1.406572	-0.587200	H	3.133964	1.395761	-0.611220	H	3.603473	1.410074	-0.575266
H	-2.765897	-1.406572	-0.587200	H	-3.133964	-1.395761	-0.611220	H	-3.603473	-1.410074	-0.575266
H	-3.647019	-0.889474	0.844215	H	-4.090291	-0.903957	0.777616	H	-4.602767	-0.889207	0.771423
H	-2.765897	1.406572	0.587200	H	-3.133964	1.395761	0.611220	H	-3.603473	1.410074	0.575266
H	-3.647019	0.889474	-0.844215	H	-4.090291	0.903957	-0.777616	H	-4.602767	0.889207	-0.771423

Table S6. B3LYP optimized geometries (Cartesian coordinates in Å) for M(12C4) (M = Li, Na, K).

Li(12C4)				Na(12C4)				K(12C4)			
O	0.000000	1.971267	0.440001	O	0.000000	1.602371	0.175886	O	0.000000	1.715542	-0.005944
O	-1.616245	0.000000	-0.273953	O	-2.223954	0.000000	-0.779035	O	-2.088820	0.000000	-1.006851
O	1.616245	-0.000000	-0.273953	O	2.223954	-0.000000	-0.779035	O	2.088820	-0.000000	-1.006851
O	-0.000000	-1.971267	0.440001	O	-0.000000	-1.602371	0.175886	O	-0.000000	-1.715542	-0.005944
C	1.226127	2.317584	-0.215327	C	1.195947	2.134894	-0.380317	C	1.199138	2.183466	-0.610009
C	-2.246987	1.230635	0.082880	C	-2.358597	1.217546	-0.065917	C	-2.326123	1.214841	-0.319948
C	2.246987	1.230635	0.082880	C	2.358597	1.217546	-0.065917	C	2.326123	1.214841	-0.319948
C	-2.246987	-1.230635	0.082880	C	-2.358597	-1.217546	-0.065917	C	-2.326123	-1.214841	-0.319948
C	2.246987	-1.230635	0.082880	C	2.358597	-1.217546	-0.065917	C	2.326123	-1.214841	-0.319948
C	-1.226127	-2.317584	-0.215327	C	-1.195947	-2.134894	-0.380317	C	-1.199138	-2.183466	-0.610009
C	1.226127	-2.317584	-0.215327	C	1.195947	-2.134894	-0.380317	C	1.199138	-2.183466	-0.610009
C	-1.226127	2.317584	-0.215327	C	-1.195947	2.134894	-0.380317	C	-1.199138	2.183466	-0.610009
H	1.589521	3.283936	0.145836	H	1.397151	3.133366	0.027943	H	1.461652	3.177649	-0.227231
H	1.059265	2.381779	-1.293027	H	1.089929	2.220612	-1.466441	H	1.064238	2.256135	-1.693476
H	-2.511476	1.222084	1.145654	H	-2.411226	1.038187	1.013908	H	-2.407457	1.046597	0.760207
H	-3.154319	1.391247	-0.512404	H	-3.288053	1.718004	-0.360115	H	-3.271296	1.661898	-0.650683
H	3.154319	1.391247	-0.512404	H	3.288053	1.718004	-0.360115	H	3.271296	1.661898	-0.650683
H	2.511476	1.222084	1.145654	H	2.411226	1.038187	1.013908	H	2.407457	1.046597	0.760207
H	-3.154319	-1.391247	-0.512404	H	-3.288053	-1.718004	-0.360115	H	-3.271296	-1.661898	-0.650683
H	-2.511476	-1.222084	1.145654	H	-2.411226	-1.038187	1.013908	H	-2.407457	-1.046597	0.760207
H	2.511476	-1.222084	1.145654	H	2.411226	-1.038187	1.013908	H	2.407457	-1.046597	0.760207
H	3.154319	-1.391247	-0.512404	H	3.288053	-1.718004	-0.360115	H	3.271296	-1.661898	-0.650683
H	-1.589521	-3.283936	0.145836	H	-1.397151	-3.133366	0.027943	H	-1.461652	-3.177649	-0.227231
H	-1.059265	-2.381779	-1.293027	H	-1.089929	-2.220612	-1.466441	H	-1.064238	-2.256135	-1.693476
H	1.059265	-2.381779	-1.293027	H	1.089929	-2.220612	-1.466441	H	1.064238	-2.256135	-1.693476
H	1.589521	-3.283936	0.145836	H	1.397151	-3.133366	0.027943	H	1.461652	-3.177649	-0.227231
H	-1.589521	3.283936	0.145836	H	-1.397151	3.133366	0.027943	H	-1.461652	3.177649	-0.227231
H	-1.059265	2.381779	-1.293027	H	-1.089929	2.220612	-1.466441	H	-1.064238	2.256135	-1.693476
Li	0.000000	0.000000	0.859242	Na	0.000000	0.000000	2.136257	K	0.000000	0.000000	2.408864

Table S7. B3LYP optimized geometries (Cartesian coordinates in Å) for M(15C5) (M = Li, Na, K).

Li(15C5)				Na(15C5)				K(15C5)			
O	2.139769	0.694433	-0.218129	O	-2.206119	0.788214	0.375442	O	0.057777	2.054807	-0.498897
O	1.298047	-1.763754	0.134924	O	-1.435516	-1.831693	-0.151011	O	2.394192	0.706759	0.167110
O	0.003242	2.100764	-0.000750	O	0.049856	2.137613	-0.004659	O	-2.353748	0.858045	0.410184
O	-1.304223	-1.760661	-0.136690	O	1.284206	-1.808138	0.233482	O	1.300820	-1.758285	-0.436311
O	-2.137823	0.701011	0.218221	O	2.326774	0.708059	-0.227816	O	-1.474291	-1.823035	0.001277
C	0.701099	-2.994277	-0.262201	C	-0.777095	-2.966599	0.389535	C	3.191073	-0.336727	-0.375367
C	1.204319	2.863950	-0.120324	C	-1.133123	2.904434	0.175848	C	-2.303504	1.842829	-0.613636
C	-0.710388	-2.991849	0.263010	C	0.631478	-3.009543	-0.159687	C	2.626687	-1.670967	0.060925
C	3.114595	-0.262555	0.179424	C	-3.146698	-0.179589	-0.067624	C	1.238207	2.773132	-0.170372
C	2.641548	-1.604610	-0.313227	C	-2.694344	-1.531814	0.435099	C	2.430458	1.926379	-0.556372
C	-1.195406	2.867366	0.120605	C	1.283395	2.843089	0.012969	C	-3.242391	-0.229838	0.185037
C	-2.646450	-1.596439	0.313279	C	2.619637	-1.660913	-0.234446	C	0.618894	-2.969223	-0.155669
C	-2.341843	1.996314	-0.335003	C	2.355733	1.906662	0.532185	C	-2.632583	-1.337502	-0.655895
C	-3.115422	-0.252965	-0.179369	C	3.138639	-0.339567	0.286764	C	-0.782767	-2.842670	-0.707820
C	2.347912	1.989134	0.335262	C	-2.315524	2.057130	-0.252309	C	-1.150913	2.778301	-0.327368
H	3.302289	2.407546	-0.008359	H	-3.248273	2.561066	0.034077	H	-1.190480	3.628059	-1.020897
H	1.257046	-3.842328	0.155596	H	-1.304601	-3.887824	0.114200	H	4.229620	-0.247121	-0.035639
H	0.708353	-3.072567	-1.354586	H	-0.749305	-2.895143	1.482968	H	3.177667	-0.281403	-1.468842
H	1.157507	3.757708	0.509688	H	-1.111763	3.810344	-0.440134	H	-3.240972	2.411201	-0.631458
H	1.327254	3.172690	-1.162840	H	-1.219622	3.196335	1.228009	H	-2.157482	1.382351	-1.595941
H	-1.268578	-3.839465	-0.152701	H	1.155997	-3.883572	0.246117	H	3.252027	-2.476423	-0.345742
H	-0.717551	-3.067670	1.355582	H	0.611676	-3.088203	-1.253308	H	2.634640	-1.757251	1.155845
H	3.205755	-0.266078	1.271016	H	-3.195304	-0.186993	-1.162948	H	1.257697	3.004014	0.902735
H	4.092332	-0.020319	-0.254706	H	-4.147519	0.042350	0.324661	H	1.282986	3.720288	-0.722926
H	2.673660	-1.652034	-1.406851	H	-2.601584	-1.513240	1.527022	H	2.393716	1.719070	-1.631328
H	3.276910	-2.400640	0.093187	H	-3.436153	-2.291463	0.161201	H	3.352430	2.480572	-0.341334
H	-1.146433	3.761703	-0.508404	H	1.228373	3.712125	0.676200	H	-4.169776	0.116118	-0.284252
H	-1.316705	3.175265	1.163575	H	1.520680	3.188562	-0.998475	H	-3.487042	-0.620691	1.173423
H	-2.677184	-1.642931	1.406991	H	2.641080	-1.678617	-1.330837	H	0.588856	-3.156661	0.925585
H	-3.285288	-2.390467	-0.091607	H	3.252641	-2.474551	0.141516	H	1.121633	-3.819517	-0.634888
H	-3.294806	2.417868	0.008691	H	3.335197	2.394631	0.455079	H	-3.376739	-2.136224	-0.774442
H	-2.363074	1.925916	-1.428169	H	2.165351	1.675111	1.586648	H	-2.366984	-0.977344	-1.657473
H	-3.206654	-0.256250	-1.270967	H	3.095998	-0.338733	1.381315	H	-0.729194	-2.586396	-1.771736
H	-4.092478	-0.007907	0.254707	H	4.181797	-0.203225	-0.020906	H	-1.308469	-3.799545	-0.606734
H	2.368812	1.918446	1.428407	H	-2.307143	1.933006	-1.342584	H	-1.228841	3.164742	0.696053
Li	0.002319	0.020916	0.000798	Na	0.018754	-0.014923	-1.029394	K	0.031987	0.017028	1.653806

Table S8. B3LYP optimized geometries (Cartesian coordinates in Å) for M(18C6) (M = Na, K).

Na(18C6)				K(18C6)			
H	-0.058165	3.274171	3.287097	H	1.197439	4.491721	-0.063612
O	0.095314	1.399580	2.424377	O	0.000000	2.808176	0.077795
O	-0.254177	2.822371	0.000000	O	2.437748	1.407434	-0.262079
O	-0.258328	-1.411690	2.444172	O	-2.437748	1.407434	-0.262079
O	0.095314	1.399580	-2.424377	O	2.431952	-1.404088	0.077795
O	0.098702	-2.799736	0.000000	O	-2.431952	-1.404088	0.077795
O	-0.258328	-1.411690	-2.444172	O	-0.000000	-2.814869	-0.262079
C	-0.366962	0.690133	3.559229	C	-1.186159	3.440177	-0.377835
C	0.246348	3.425861	-1.181733	C	3.569108	0.692331	0.217760
C	0.244585	-2.735960	2.376503	C	-3.569108	0.692331	0.217760
C	-0.361105	2.739050	-2.377628	C	3.572360	-0.692844	-0.377835
C	-0.359325	-3.429345	1.182611	C	-3.572360	-0.692844	-0.377835
C	0.246348	3.425861	1.181733	C	2.384131	2.744773	0.217760
C	0.238413	-0.689885	3.559193	C	-2.384131	2.744773	0.217760
C	-0.366962	0.690133	-3.559229	C	2.386201	-2.747333	-0.377835
C	-0.359325	-3.429345	-1.182611	C	-2.386201	-2.747333	-0.377835
C	0.238413	-0.689885	-3.559193	C	1.184978	-3.437104	0.217760
C	0.244585	-2.735960	-2.376503	C	-1.184978	-3.437104	0.217760
C	-0.361105	2.739050	2.377628	C	1.186159	3.440177	-0.377835
H	-1.461955	0.621732	3.545514	H	-1.234455	3.407463	-1.472746
H	-0.067024	1.209815	4.478572	H	-1.197439	4.491721	-0.063612
H	1.338826	3.339816	-1.217298	H	3.541481	0.630922	1.312142
H	-0.021157	4.490839	-1.205647	H	4.493411	1.207306	-0.075686
H	-0.023413	-3.289820	3.286294	H	-4.493411	1.207306	-0.075686
H	1.337174	-2.721669	2.285934	H	-3.541481	0.630922	1.312142
H	-1.456039	2.766291	-2.312210	H	3.568177	-0.634662	-1.472746
H	-0.058165	3.274171	-3.287097	H	4.488664	-1.208848	-0.063612
H	-0.054750	-4.484038	1.192259	H	-4.488664	-1.208848	-0.063612
H	-1.454435	-3.387992	1.236445	H	-3.568177	-0.634662	-1.472746
H	-0.021157	4.490839	1.205647	H	3.292263	3.287756	-0.075686
H	1.338826	3.339816	1.217298	H	2.317135	2.751552	1.312142
H	1.331187	-0.617509	3.507125	H	-2.317135	2.751552	1.312142
H	-0.033601	-1.200717	4.492686	H	-3.292263	3.287756	-0.075686
H	-0.067024	1.209815	-4.478572	H	3.291225	-3.282873	-0.063612
H	-1.461955	0.621732	-3.545514	H	2.333722	-2.772801	-1.472746
H	-1.454435	-3.387992	-1.236445	H	-2.333722	-2.772801	-1.472746
H	-0.054750	-4.484038	-1.192259	H	-3.291225	-3.282873	-0.063612
H	-0.033601	-1.200717	-4.492686	H	1.201148	-4.495061	-0.075686
H	1.331187	-0.617509	-3.507125	H	1.224346	-3.382473	1.312142
H	-0.023413	-3.289820	-3.286294	H	-1.201148	-4.495061	-0.075686
H	1.337174	-2.721669	-2.285934	H	-1.224346	-3.382473	1.312142
H	-1.456039	2.766291	2.312210	H	1.234455	3.407463	-1.472746
Na	0.854117	0.001145	0.000000	K	0.000000	0.000000	0.630787

Table S9. B3LYP harmonic vibrational frequencies (cm^{-1}) for $M(en)_2$, M(12C4), M(15C5), and M(18C6) (M = Li, Na, K).

$Li(en)_2$	$Na(en)_2$	$K(en)_2$	Li(12C4)	Na(12C4)	K(12C4)	Li(15C5)	Na(15C5)	K(15C5)	Na(18C6)	K(18C6)
41.5	14.8	-6.7	65.5	50.5	48.6	26.6	44.3	52.8	-31.0	37.2
42.5	17.0	-3.6	111.4	57.4	56.8	47.9	54.7	54.8	-28.3	37.2
50.2	17.3	-2.5	138.7	92.0	58.9	55.2	63.2	80.0	34.8	49.7
116.3	84.0	63.3	154.3	103.4	74.5	90.6	71.1	83.7	35.2	70.2
118.4	89.3	70.6	186.7	103.5	79.0	94.1	90.6	89.1	58.4	86.2
128.2	102.4	84.0	203.1	117.8	118.9	121.7	119.7	96.6	59.4	86.2
232.7	200.0	137.0	205.3	151.3	155.4	136.7	141.1	116.6	59.7	113.9
244.9	204.3	141.2	216.9	158.9	155.5	137.3	145.7	129.9	66.9	116.8
313.2	206.6	156.8	256.3	171.1	178.1	160.2	163.4	142.4	104.9	116.9
315.4	227.6	194.8	261.9	211.4	223.3	172.7	169.3	160.3	131.4	134.8
320.5	259.5	202.5	300.8	222.7	235.0	174.8	179.9	170.4	131.6	134.8
339.3	266.6	221.9	314.1	261.1	247.3	202.9	185.1	185.0	135.9	140.5
388.2	307.3	267.6	330.9	308.3	309.2	219.7	202.0	204.8	145.4	146.6
413.2	310.6	286.3	350.9	314.8	314.8	224.1	210.1	215.2	145.9	146.6
413.9	321.1	290.8	368.4	338.0	348.2	238.0	231.9	232.6	162.9	167.0
449.0	353.3	322.9	429.2	391.0	373.6	248.7	239.8	243.1	210.4	219.1
526.2	355.1	323.2	455.5	407.5	393.2	278.3	254.6	288.2	212.8	222.5
538.2	512.0	501.0	523.4	514.7	519.2	299.8	296.6	298.9	233.4	234.6
554.8	519.9	508.2	535.0	526.5	527.2	341.8	330.7	324.9	234.1	234.6
828.9	824.2	813.9	538.1	526.8	527.5	343.6	339.4	330.6	243.2	247.9
839.1	824.4	818.6	569.5	538.4	544.7	345.3	343.5	346.4	244.6	247.9
861.9	849.9	847.1	824.4	813.5	816.6	350.6	346.4	380.3	264.6	263.7
862.4	850.4	848.3	829.4	821.3	825.2	544.3	529.1	517.0	311.6	311.6
911.8	902.2	885.1	832.7	830.4	829.7	555.1	541.0	537.3	311.8	311.6
936.4	905.0	889.5	850.2	848.1	846.1	556.1	548.2	540.6	350.6	345.5
977.0	970.9	968.6	910.0	917.6	919.2	562.1	552.9	552.4	358.1	356.1
979.8	971.0	968.9	931.5	919.7	923.2	585.1	563.4	575.4	358.7	356.1
999.7	990.5	984.1	937.0	931.1	930.2	824.5	821.5	814.4	528.7	528.9
1000.8	994.9	987.6	938.4	942.0	938.5	841.5	836.8	835.8	528.9	528.9
1045.1	1048.4	1049.9	1018.0	1029.4	1035.7	850.6	844.8	838.1	535.4	537.3
1048.1	1048.6	1050.3	1018.6	1046.7	1048.7	852.4	847.2	847.3	550.2	546.7
1097.0	1104.6	1109.7	1036.5	1065.8	1060.7	899.1	872.5	862.7	550.2	546.7
1097.3	1104.9	1109.8	1069.0	1069.2	1061.5	926.4	933.0	924.7	587.4	582.9
1111.0	1113.6	1113.9	1080.6	1088.8	1088.5	960.9	941.8	934.5	840.7	837.4
1113.8	1113.7	1114.9	1093.9	1119.7	1120.0	961.9	943.2	941.9	840.8	837.4
1291.9	1291.1	1289.3	1106.6	1120.6	1123.5	974.7	959.6	953.9	849.1	844.8
1293.6	1291.4	1289.7	1113.5	1122.0	1125.2	982.2	968.4	960.4	851.6	849.6
1302.3	1307.1	1308.3	1133.9	1152.6	1157.4	1058.6	1055.6	1046.2	851.8	849.6
1302.5	1307.6	1308.6	1147.6	1163.8	1166.4	1058.9	1057.1	1058.1	879.3	880.2
1349.5	1350.3	1349.3	1147.6	1183.1	1182.9	1068.7	1058.0	1060.7	932.8	929.9
1350.1	1351.4	1350.6	1172.4	1184.3	1184.3	1080.2	1093.7	1084.6	948.0	943.5
1407.7	1410.1	1412.0	1240.7	1253.2	1251.0	1099.6	1098.0	1094.1	962.4	959.1
1408.1	1411.9	1413.7	1255.6	1270.5	1270.0	1103.7	1101.9	1098.5	962.4	959.1
1423.9	1425.9	1428.1	1260.6	1277.1	1274.4	1104.3	1113.5	1113.6	978.3	974.7
1423.9	1426.5	1428.8	1268.5	1290.5	1289.6	1110.1	1116.6	1117.0	978.4	974.7
1498.7	1499.8	1502.2	1269.7	1296.2	1294.5	1119.9	1128.9	1129.0	1070.9	1067.5
1499.8	1501.0	1502.8	1274.4	1304.6	1300.6	1132.6	1137.2	1135.5	1071.0	1067.5
1500.6	1501.4	1502.9	1282.1	1308.8	1304.4	1138.6	1139.4	1143.6	1078.9	1076.5
1500.9	1501.6	1503.1	1285.8	1313.1	1307.7	1142.2	1146.5	1154.3	1099.9	1097.2
1624.0	1631.2	1640.3	1367.9	1377.6	1375.4	1146.2	1154.0	1160.1	1099.9	1098.1
1626.6	1632.6	1640.6	1382.2	1390.1	1389.7	1164.9	1168.5	1165.1	1106.2	1098.1
1632.2	1636.0	1642.4	1382.8	1393.9	1390.6	1166.2	1172.2	1172.6	1109.8	1107.3
1633.8	1636.5	1643.1	1390.0	1397.6	1395.5	1255.7	1253.8	1253.1	1127.1	1116.9
2990.1	2981.1	2968.8	1418.9	1424.4	1424.0	1259.4	1257.3	1256.9	1127.1	1116.9
2990.3	2981.1	2968.9	1429.1	1427.5	1428.1	1267.5	1268.1	1263.0	1132.6	1125.9
3000.8	2994.3	2984.4	1429.5	1441.3	1439.0	1268.4	1269.5	1267.6	1132.7	1125.9
3001.8	2995.1	2985.2	1440.4	1447.0	1445.6	1271.1	1273.8	1273.5	1134.0	1132.0
3052.4	3046.5	3038.7	1488.6	1487.1	1486.1	1276.5	1282.2	1288.1	1152.8	1150.8
3053.0	3047.1	3039.1	1488.6	1487.7	1486.7	1284.7	1286.4	1290.2	1152.9	1150.8
3067.2	3062.1	3056.0	1489.0	1491.6	1493.3	1291.4	1295.8	1301.9	1160.4	1151.5
3067.8	3062.7	3056.4	1490.3	1491.9	1493.5	1295.0	1299.1	1303.7	1160.5	1151.5

3391.2	3404.3	3431.1	1496.4	1507.1	1508.7	1296.1	1303.3	1320.2	1166.9	1158.9
3395.1	3406.2	3431.8	1496.9	1508.9	1509.7	1375.4	1372.4	1372.6	1166.9	1165.3
3397.3	3409.8	3433.8	1509.6	1509.8	1511.7	1387.0	1382.7	1382.8	1252.9	1254.4
3412.6	3420.9	3438.8	1511.0	1514.2	1514.8	1388.6	1385.8	1385.5	1259.5	1260.7
3463.2	3479.8	3507.2	2967.1	2970.2	2966.7	1401.5	1397.4	1396.7	1259.6	1260.7
3464.3	3480.0	3507.3	2967.2	2970.8	2967.3	1403.3	1400.1	1406.4	1268.6	1269.6
3470.0	3485.1	3510.3	2971.4	2975.5	2974.4	1432.7	1429.5	1420.2	1268.7	1269.6
3473.5	3485.8	3510.3	2972.9	2978.7	2976.0	1434.3	1430.4	1430.1	1272.0	1273.0
			3007.1	2978.7	2979.3	1452.1	1447.1	1439.4	1291.8	1290.9
			3008.4	2984.0	2983.0	1454.6	1450.0	1450.6	1298.9	1298.5
			3008.7	2984.9	2984.8	1464.2	1459.8	1456.7	1298.9	1298.5
			3010.9	2987.0	2987.0	1493.1	1491.8	1485.7	1310.0	1310.0
			3016.4	3010.7	3004.3	1494.1	1492.1	1489.9	1310.1	1310.0
			3019.2	3011.9	3005.1	1494.4	1492.7	1492.2	1314.2	1314.0
			3019.3	3013.5	3007.0	1496.9	1493.7	1495.9	1374.6	1375.5
			3020.3	3014.1	3007.0	1497.4	1494.3	1498.9	1383.3	1383.9
			3054.9	3028.4	3031.1	1503.2	1505.0	1501.9	1383.3	1383.9
			3055.7	3029.6	3031.6	1503.4	1505.7	1510.5	1398.0	1398.8
			3056.0	3029.8	3031.8	1507.1	1509.1	1512.7	1398.0	1398.8
			3056.4	3030.3	3032.1	1508.5	1512.7	1514.3	1405.1	1405.1
						1509.4	1513.8	1515.4	1428.8	1430.0
						2966.6	2954.3	2953.3	1441.1	1441.2
						2967.5	2966.0	2960.9	1441.1	1441.2
						2972.2	2968.3	2962.1	1462.1	1460.6
						2973.8	2971.4	2968.4	1462.1	1460.6
						2975.1	2976.2	2970.9	1471.6	1469.8
						2978.3	2978.8	2978.1	1488.6	1490.3
						2981.3	2981.8	2982.2	1489.0	1491.2
						2983.3	2985.0	2983.4	1489.0	1491.2
						2988.0	2987.7	2987.2	1491.9	1492.9
						2998.4	2992.7	2995.2	1492.1	1492.9
						3007.7	2997.9	2996.1	1492.2	1493.8
						3008.6	3003.0	2997.5	1505.6	1506.2
						3011.3	3005.0	2998.1	1505.7	1507.5
						3011.6	3005.3	3004.9	1506.8	1507.5
						3012.4	3011.5	3007.5	1511.8	1511.2
						3023.6	3018.1	3020.0	1511.8	1511.2
						3024.8	3021.9	3021.3	1512.3	1512.3
						3024.9	3024.6	3025.4	2958.9	2961.8
						3034.6	3025.4	3030.0	2959.7	2962.2
						3035.3	3039.5	3074.4	2959.8	2962.2
									2962.4	2965.6
									2962.4	2965.6
									2964.5	2967.1
									2968.6	2972.3
									2971.0	2973.6
									2971.1	2973.6
									2975.7	2978.9
									2975.7	2978.9
									2978.3	2980.8
									2992.9	2996.6
									2993.2	2997.1
									2993.3	2997.1
									2996.6	3000.6
									2996.6	3000.6
									2997.0	3000.8
									3010.6	3013.0
									3010.8	3013.0
									3011.0	3013.3
									3012.5	3015.1
									3012.5	3015.4
									3012.7	3015.4

Table S10. Vertical excitation energies (eV) for $Li(en)_2$ at the KT, D2, P3, P3+, and EOM-EA-CCSD levels of theory.

Occupied orbital	H: DATZ, Li,C,N: TZ				
	KT	D2	P3	P3+	EOM-EA-CCSD
11^2a	0.000	0.000	0.000	0.000	0.000
9^2b_1	0.262	0.355	0.350	0.350	0.369
9^2b_2	0.310	0.422	0.416	0.416	0.436
10^2b_3	0.483	0.613	0.607	0.608	0.621
10^2b_2	0.809	1.017	1.010	1.011	1.046
12^2a	0.826	1.029	1.021	1.022	1.059
13^2a	0.812	1.054	1.047	1.047	1.106
11^2b_3	0.819	1.057	1.049	1.050	1.100
10^2b_1	0.854	1.087	1.079	1.079	1.127
14^2a	1.205	1.384	1.387	1.386	1.419
11^2b_2	1.231	1.466	1.462	1.462	1.477
11^2b_1	1.230	1.469	1.465	1.465	1.478
12^2b_3	1.244	1.506	1.502	1.502	1.524
13^2b_3	1.308	1.620	1.614	1.614	1.668
15^2a	1.343	1.620	1.616	1.616	1.682
12^2b_1	1.385	1.620	1.618	1.618	1.672
12^2b_2	1.397	1.643	1.640	1.640	1.700
13^2b_1	1.347	1.670	1.665	1.665	1.721
14^2b_3	1.604	1.757	1.757	1.757	1.779
13^2b_2	1.559	1.870	1.865	1.865	1.840
15^2b_3	1.695	1.895	1.890	1.891	
16^2a	1.691	1.897	1.893	1.893	
14^2b_2	1.714	1.901	1.899	1.899	
17^2a	1.722	1.909	1.904	1.904	
14^2b_1	1.763	1.942	1.937	1.937	
15^2b_1	2.067	2.244	2.239	2.239	
16^2b_3	2.104	2.244	2.242	2.242	
15^2b_2	2.072	2.251	2.245	2.245	
18^2a	2.184[a]	2.360	2.355	2.356	
16^2b_2	2.208[a]	2.399	2.389	2.390	
17^2b_3	2.217[a]	2.415	2.408	2.408	
16^2b_1	2.250[a]	2.470	2.464	2.464	

[a] States are not bound with respect to the ionization energy at KT level of theory.

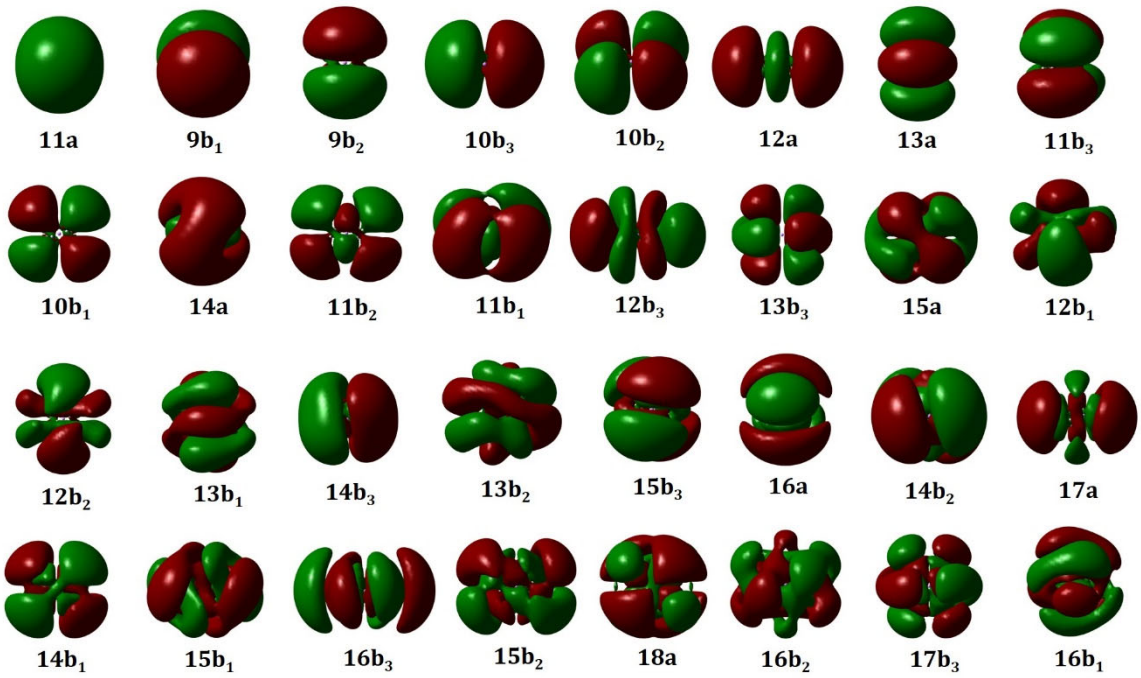

Figure S1. Dyson orbitals for vertical electron attachment to $Li(en)_2^+$.

Table S11. Vertical excitation energies (eV) for $Na(en)_2$ at the KT, D2, P3, and P3+ levels of theory.

Occupied orbital	H: DATZ, Na,C,N: TZ			
	KT	D2	P3	P3+
12^2a	0.000	0.000	0.000	0.000
10^2b_1	0.279	0.382	0.376	0.376
9^2b_2	0.320	0.439	0.433	0.434
12^2b_3	0.517	0.645	0.641	0.641
13^2a	0.811	0.996	0.990	0.991
10^2b_2	0.810	1.008	1.004	1.004
11^2b_1	0.856	1.078	1.072	1.073
13^2b_3	0.841	1.087	1.081	1.082
14^2a	0.837	1.089	1.083	1.083
15^2a	1.174	1.353	1.356	1.356
11^2b_2	1.184	1.407	1.404	1.405
12^2b_1	1.184	1.410	1.406	1.407
14^2b_3	1.223	1.474	1.471	1.471
15^2b_3	1.292	1.593	1.589	1.589
16^2a	1.323	1.598	1.595	1.595
12^2b_2	1.365	1.630	1.628	1.628
13^2b_1	1.345	1.635	1.633	1.633
14^2b_1	1.375	1.664	1.662	1.662
16^2b_3	1.517	1.716	1.717	1.717
13^2b_2	1.579	1.866	1.864	1.864
17^2a	1.746	1.906	1.904	1.904
18^2a	1.712	1.918	1.914	1.915
17^2b_3	1.733	1.925	1.920	1.921
15^2b_1	1.768	1.926	1.924	1.924
14^2b_2	1.751	1.953	1.952	1.952
16^2b_1	2.000	2.187	2.183	2.184
18^2b_3	2.034	2.210	2.206	2.206
15^2b_2	2.048	2.225	2.219	2.220
19^2a	2.138[a]	2.303	2.301	2.301
19^2b_3	2.179[a]	2.380	2.375	2.376
16^2b_2	2.216[a]	2.406	2.397	2.398
17^2b_1	2.251[a]	2.456	2.451	2.451

[a] States are not bound with respect to the ionization energy at KT level of theory.

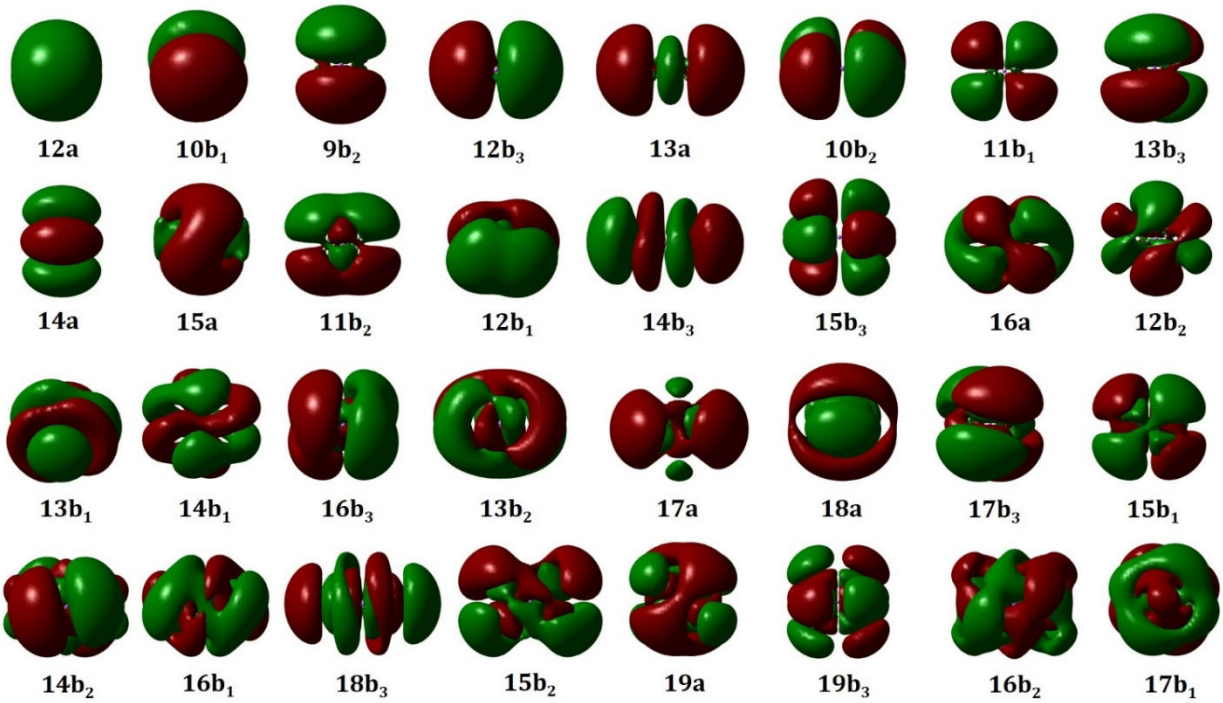

Figure S2. Dyson orbitals for vertical electron attachment to $Na(en)_2^+$.

Table S12. Vertical excitation energies (eV) for $K(en)_2$ at the KT, D2, P3, and P3+ levels of theory.

Occupied orbital	H: DATZ, K,C,N: TZ			
	KT	D2	P3	P3+
13^2a	0.000	0.000	0.000	0.000
11^2b_2	0.362	0.455	0.451	0.451
11^2b_1	0.353	0.468	0.467	0.468
12^2b_3	0.616	0.710	0.711	0.712
14^2a	0.843	0.997	0.996	0.996
12^2b_1	0.879	1.032	1.031	1.032
12^2b_2	0.908	1.081	1.081	1.081
13^2b_3	0.894	1.107	1.105	1.106
15^2a	0.903	1.112	1.110	1.110
16^2a	1.167	1.361	1.364	1.365
13^2b_1	1.188	1.399	1.400	1.400
13^2b_2	1.205	1.413	1.412	1.413
14^2b_3	1.257	1.462	1.462	1.463
17^2a	1.349	1.590	1.591	1.592
15^2b_3	1.341	1.599	1.600	1.600
14^2b_2	1.389	1.613	1.616	1.616
14^2b_1	1.391	1.640	1.642	1.642
16^2b_3	1.534	1.705	1.711	1.711
15^2b_2	1.484	1.763	1.765	1.766
15^2b_1	1.569	1.802	1.804	1.804
16^2b_2	1.709	1.858	1.861	1.861
18^2a	1.656	1.867	1.866	1.867
17^2b_3	1.668	1.876	1.876	1.876
19^2a	1.752	1.882	1.886	1.886
16^2b_1	1.774	1.948	1.951	1.951
17^2b_1	1.864	2.068	2.070	2.070
17^2b_2	2.033	2.187	2.189	2.189
18^2b_3	2.057	2.192	2.192	2.193
18^2b_1	2.138[a]	2.286	2.285	2.285
20^2a	2.123	2.301	2.301	2.301
21^2a	2.151[a]	2.300	2.302	2.302
18^2b_2	2.168[a]	2.345	2.343	2.344
19^2b_3	2.217[a]	2.390	2.390	2.390

[a] States are not bound with respect to the ionization energy at KT level of theory.

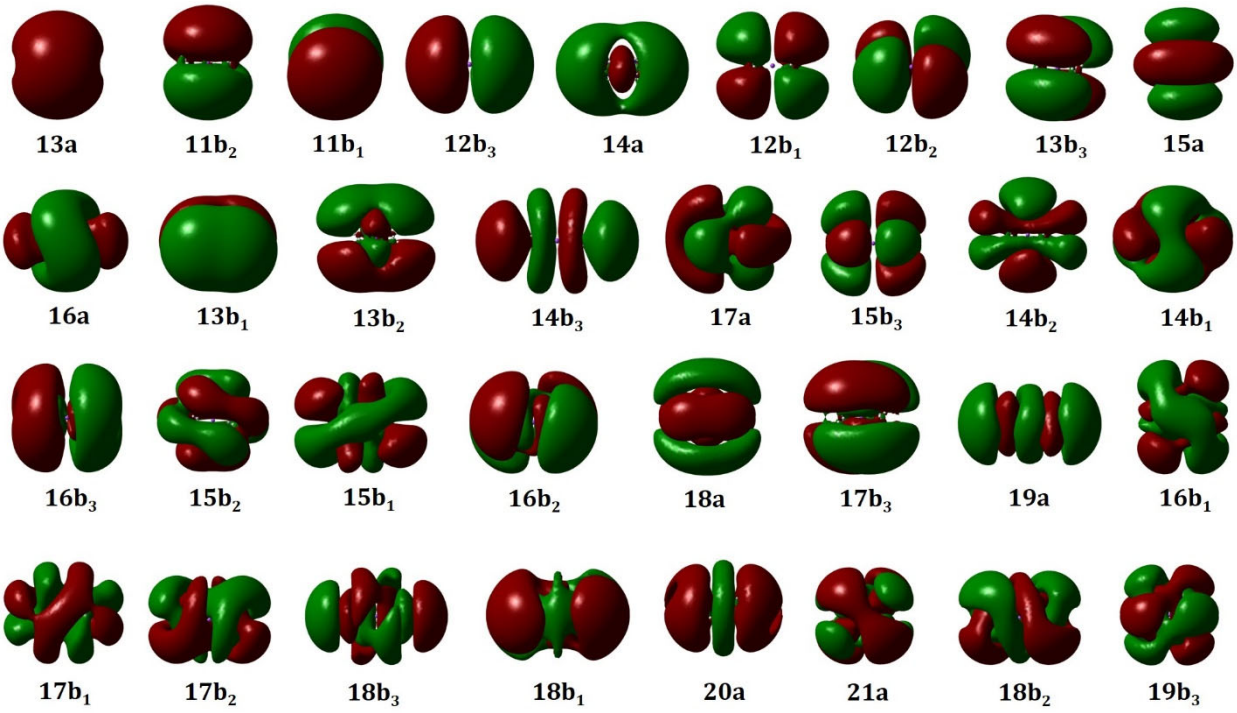

Figure S3. Dyson orbitals for vertical electron attachment to $K(en)_2^+$.

Table S13. Vertical excitation energies (eV) for Li(12C4) at the KT, D2, P3, and P3+ levels of theory.

Occupied orbital	H: DATZ, Li,C,O: TZ				H: DATZ, Li: ATZ, C,O: TZ
	KT	D2	P3	P3+	P3+
$17a_1$	0.000	0.000	0.000	0.000	0.000
$18a_1$	0.421	0.609	0.587	0.590	0.589
$13b_1$	0.488	0.681	0.654	0.656	0.657
$13b_2$	0.557	0.786	0.758	0.760	0.760
$19a_1$	0.819	1.048	1.031	1.033	1.032
$10a_2$	0.869	1.135	1.106	1.109	1.109
$20a_1$	0.881	1.155	1.126	1.129	1.126
$14b_1$	0.873	1.161	1.136	1.138	1.138
$14b_2$	0.894	1.182	1.157	1.159	1.158
$21a_1$	1.136	1.385	1.374	1.375	1.359
$15b_1$	1.308	1.612	1.592	1.594	1.560
$16b_1$	1.296	1.639	1.613	1.615	1.616
$15b_2$	1.295	1.641	1.614	1.617	1.617
$11a_2$	1.327	1.691	1.667	1.669	1.669
$16b_2$	1.356	1.712	1.690	1.692	1.673
$22a_1$	1.564	1.734	1.721	1.723	1.596
$17b_1$	1.618	1.848	1.827	1.829	1.771
$23a_1$	1.670	1.899	1.874	1.876	1.678

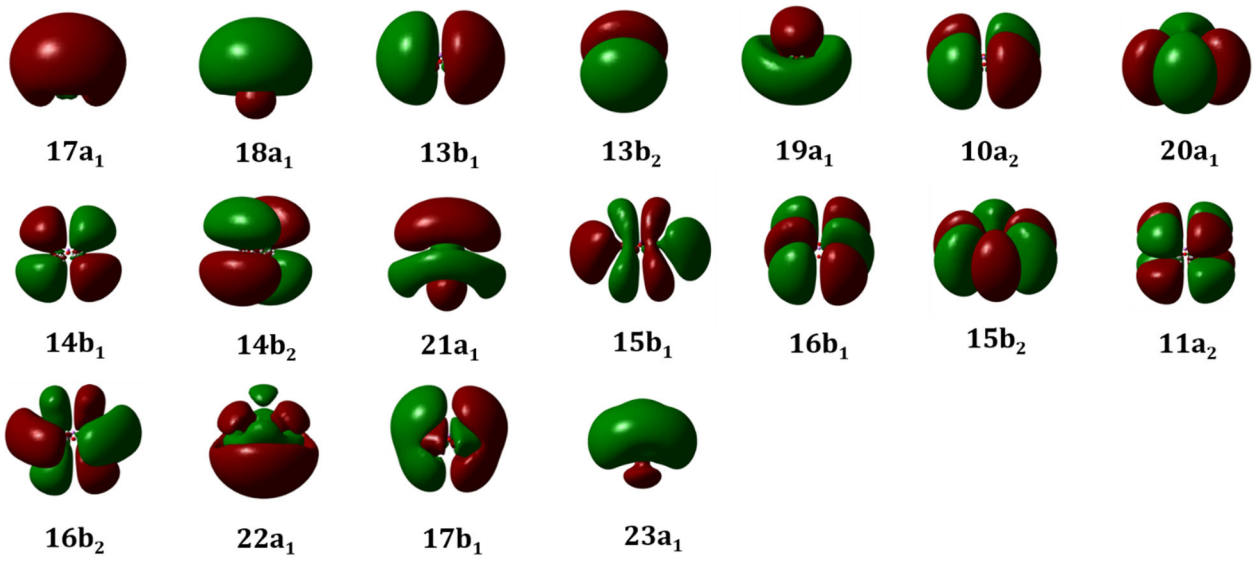

Figure S4. Dyson orbitals for vertical electron attachment to $Li(12C4)^{+}$.

Table S14. Vertical excitation energies (eV) for Na(12C4) at the KT, D2, P3, and P3+ levels of theory.

Occupied orbital	H: DATZ, Na,C,O: TZ			
	KT	D2	P3	P3+
$19a_1$	0.000	0.000	0.000	0.000
$14b_1$	1.315	1.381	1.367	1.367
$14b_2$	1.327	1.437	1.422	1.422
$20a_1$	1.679	1.880	1.858	1.858
$21a_1$	1.904	2.120	2.108	2.108
$10a_2$	1.983	2.199	2.177	2.177
$15b_2$	1.986	2.211	2.189	2.189
$22a_1$	2.028	2.236	2.214	2.214
$15b_1$	2.025	2.258	2.237	2.237
$23a_1$	2.085	2.295	2.280	2.280
$16b_1$	2.326	2.541	2.529	2.529
$16b_2$	2.361	2.622	2.608	2.608
$11a_2$	2.451	2.758	2.738	2.738
$17b_1$	2.462	2.762	2.741	2.741
$24a_1$	2.490	2.759	2.743	2.743
$17b_2$	2.462	2.765	2.744	2.744
$18b_2$	2.600	2.868	2.851	2.851
$18b_1$	2.635	2.914	2.897	2.897
$25a_1$	2.772	2.931	2.914	2.914
$12a_2$	2.804	3.049	3.031	3.031
$19b_2$	2.872	3.075	3.055	3.055
$19b_1$	2.900	3.110	3.089	3.089
$26a_1$	2.941	3.116	3.097	3.097
$27a_1$	3.003	3.167	3.152	3.152
$13a_2$	2.855	3.202	3.184	3.184
$14a_2$	3.008	3.286	3.267	3.267
$28a_1$	3.255	3.389	3.365	3.365
$20b_2$	3.193	3.437	3.417	3.417
$20b_1$	3.250	3.462	3.442	3.442
$21b_1$	3.382	3.459	3.451	3.451
$15a_2$	3.308	3.515	3.494	3.494
$29a_1$	3.447	3.523	3.518	3.518
$22b_1$	3.386	3.548	3.533	3.533
$21b_2$	3.374	3.566	3.543	3.543

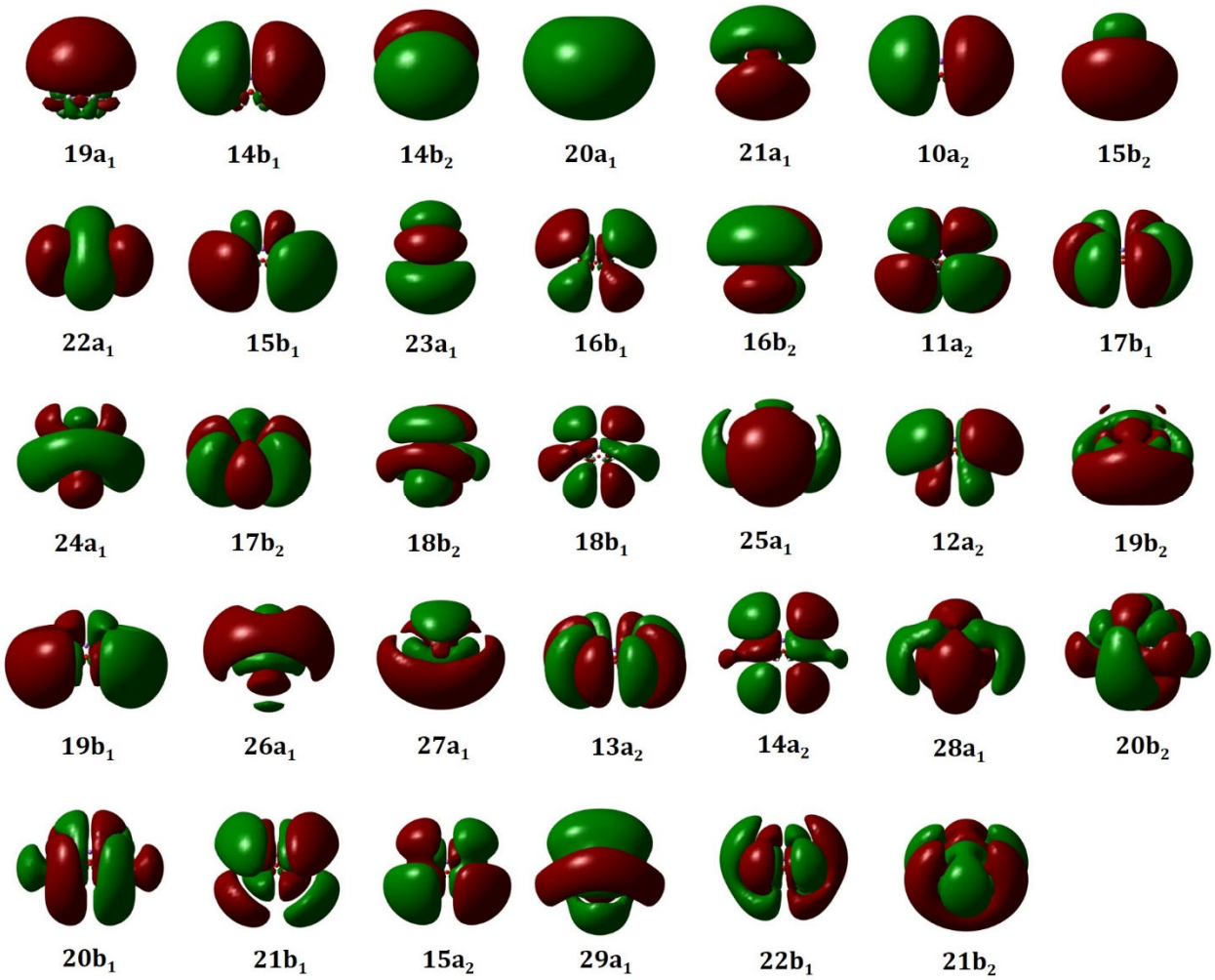

Figure S5. Dyson orbitals for vertical electron attachment to $Na(12C4)^{+}$.

Table S15. Vertical excitation energies (eV) for K(12C4) at the KT, D2, P3, and P3+ levels of theory.

Occupied orbital	H: DATZ, K,C,O: TZ			
	KT	D2	P3	P3+
$21a_1$	0.000	0.000	0.000	0.000
$15b_1$	0.998	1.019	1.012	1.012
$15b_2$	1.030	1.077	1.071	1.072
$22a_1$	1.476	1.533	1.524	1.524
$23a_1$	1.609	1.705	1.705	1.704
$10a_2$	1.704	1.780	1.770	1.771
$24a_1$	1.724	1.804	1.794	1.795
$16b_2$	1.787	1.896	1.885	1.886
$16b_1$	1.804	1.919	1.909	1.909
$25a_1$	1.839	1.948	1.942	1.942
$17b_1$	2.127	2.255	2.251	2.251
$17b_2$	2.156	2.311	2.306	2.307
$11a_2$	2.197	2.356	2.348	2.349
$26a_1$	2.216	2.371	2.365	2.365
$27a_1$	2.259	2.395	2.389	2.389
$18b_2$	2.235	2.399	2.390	2.391
$19b_2$	2.324	2.397	2.392	2.392
$18b_1$	2.248	2.414	2.405	2.405
$19b_1$	2.334	2.419	2.414	2.415
$12a_2$	2.509	2.611	2.607	2.607
$28a_1$	2.555	2.620	2.619	2.619
$20b_2$	2.564	2.715	2.709	2.710
$20b_1$	2.579	2.730	2.724	2.724
$29a_1$	2.718	2.773	2.765	2.765
$13a_2$	2.632	2.838	2.832	2.832
$30a_1$	2.831	2.865	2.860	2.861
$31a_1$	2.911	2.913	2.915	2.914
$14a_2$	2.768	2.925	2.920	2.920
$21b_2$	2.824	2.982	2.975	2.976
$21b_1$	2.886	3.008	3.001	3.001
$15a_2$	2.929	3.030	3.021	3.021
$22b_2$	2.990	3.095	3.086	3.087
$22b_1$	3.020[a]	3.118	3.111	3.112
$32a_1$	3.117[a]	3.182	3.178	3.178
$23b_1$	3.150[a]	3.199	3.187	3.188
$23b_2$	3.171[a]	3.233	3.220	3.221

[a] States are not bound at KT.

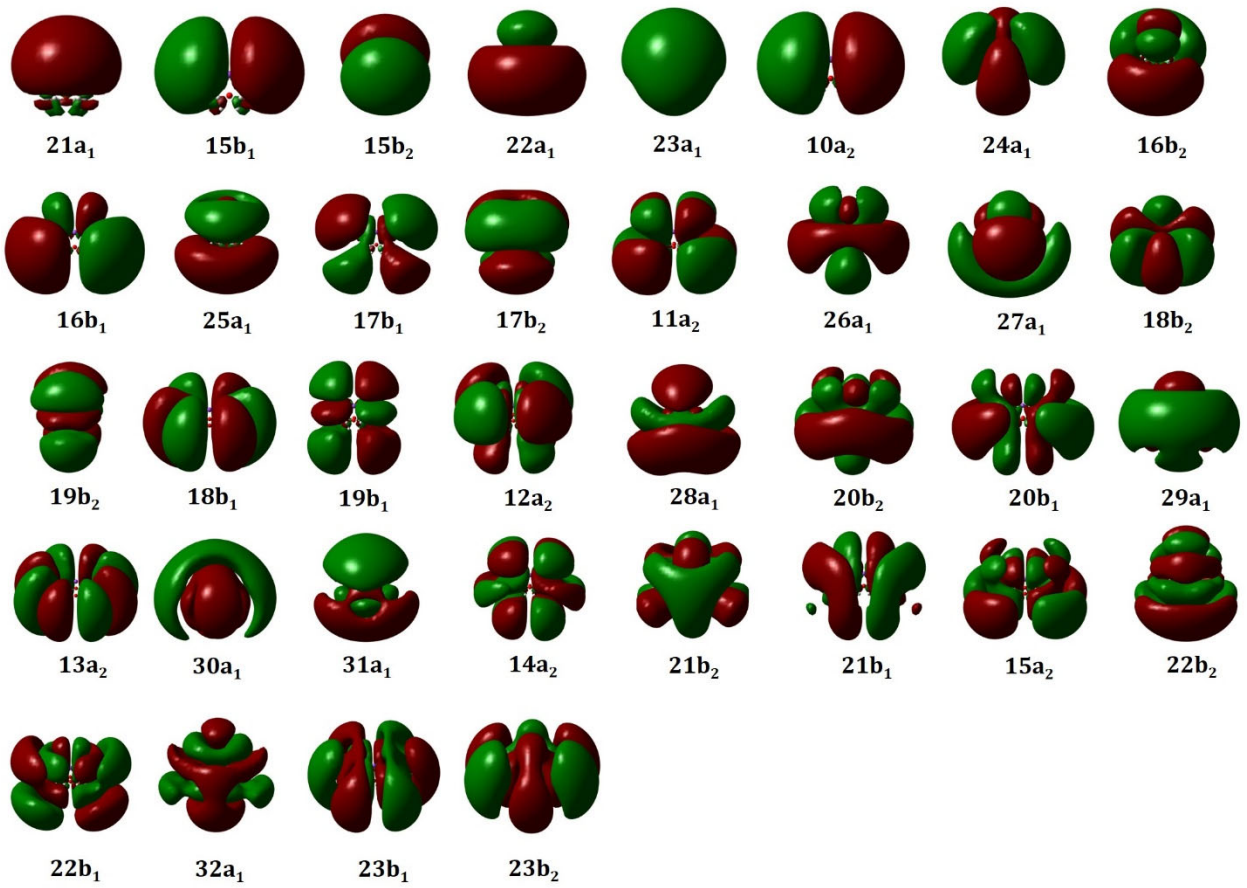

Figure S5. Dyson orbitals for vertical electron attachment to $K(12C4)^+$.

Table S16. Vertical excitation energies (eV) for Li(15C5) at the KT, D2, P3, and P3+ levels of theory.

Occupied orbital	H: DADZ, Li,C,O: DZ			
	KT	D2	P3	P3+
62a	0.000	0.000	0.000	0.000
63a	0.124	0.131	0.136	0.135
64a	0.209	0.255	0.249	0.249
65a	0.232	0.286	0.280	0.280
66a	0.510	0.597	0.592	0.592
67a	0.512	0.599	0.594	0.593
68a	0.534	0.626	0.628	0.628
69a	0.550	0.657	0.656	0.655
70a	0.555	0.663	0.662	0.661
71a	0.889	1.027	1.024	1.024
72a	0.890	1.027	1.024	1.024
73a	0.964	1.130	1.130	1.130
74a	0.972	1.130	1.133	1.132
75a	0.978	1.135	1.136	1.135
76a	1.113	1.150	1.163	1.161
77a	0.997	1.160	1.163	1.162
78a	1.510	1.304	1.334	1.331
79a	1.392	1.397	1.411	1.409
80a	1.305	1.496	1.496	1.496
81a	1.306	1.496	1.496	1.496
82a	1.569	1.550	1.548	1.548
83a	1.383	1.561	1.564	1.563
84a	1.601	1.596	1.593	1.593
85a	1.713[a]	1.700	1.700	1.700
86a	1.775[a]	1.744	1.743	1.743
87a	1.758[a]	1.745	1.745	1.745
88a	1.837[a]	1.807	1.803	1.803
89a	1.813[a]	1.816	1.819	1.818
90a	1.847[a]	1.826	1.822	1.822
91a	1.629	1.826	1.829	1.828

[a] States are not bound at KT.

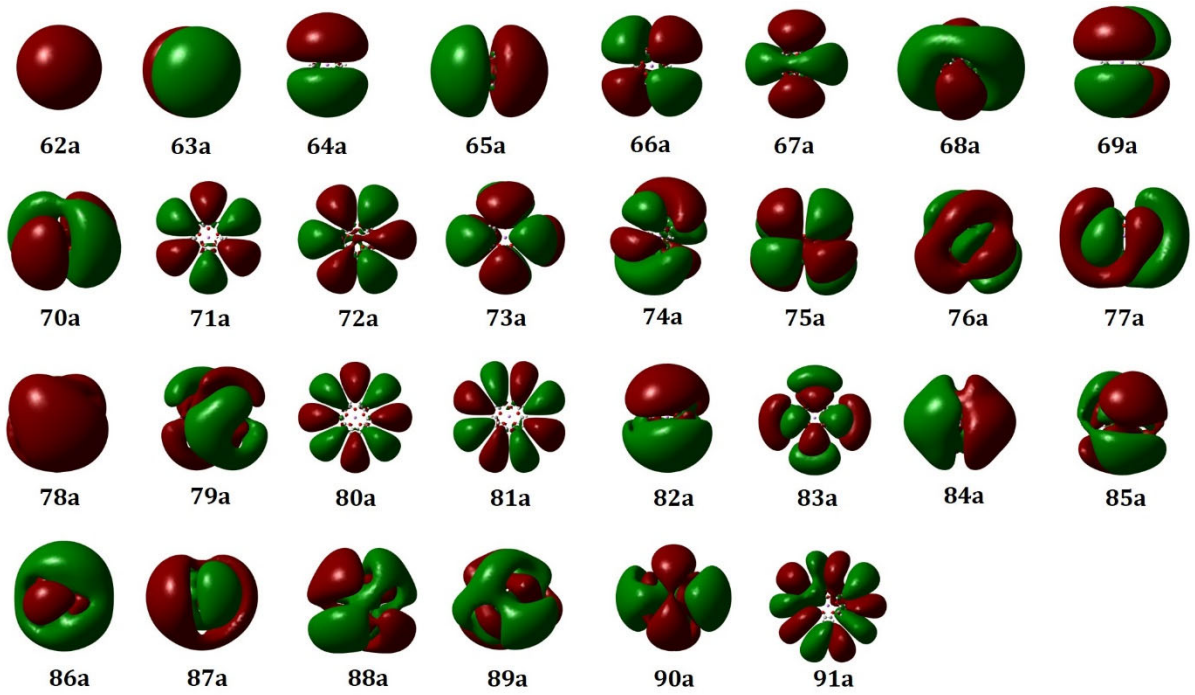

Figure S6. Dyson orbitals for vertical electron attachment to $Li(15C5)^{+}$.

Table S17. Vertical excitation energies (eV) for Na(15C5) at the KT, D2, P3, and P3+ levels of theory.

Occupied orbital	H: DADZ, Na,C,O: DZ			
	KT	D2	P3	P3+
66a	0.000	0.000	0.000	0.000
67a	0.684	0.823	0.805	0.807
68a	0.720	0.865	0.846	0.848
69a	0.770	0.936	0.916	0.918
70a	0.982	1.169	1.156	1.157
71a	1.041	1.240	1.223	1.224
72a	1.046	1.252	1.234	1.236
73a	1.077	1.283	1.263	1.265
74a	1.084	1.293	1.272	1.274
75a	1.301	1.518	1.510	1.511
76a	1.451	1.705	1.686	1.688
77a	1.454	1.709	1.691	1.692
78a	1.477	1.726	1.712	1.714
79a	1.497	1.763	1.748	1.749
80a	1.510	1.779	1.765	1.766
81a	1.533	1.797	1.783	1.784
82a	1.818	2.081	2.069	2.070
83a	1.960	2.087	2.079	2.080
84a	2.012	2.137	2.128	2.129
85a	1.865	2.166	2.151	2.153
86a	1.908	2.165	2.152	2.153
87a	1.874	2.167	2.153	2.154
88a	2.152	2.249	2.239	2.240
89a	2.214	2.299	2.284	2.286
90a	2.249[a]	2.322	2.303	2.305
91a	2.275[a]	2.362	2.345	2.346
92a	2.172	2.405	2.392	2.393
93a	2.351[a]	2.450	2.432	2.434
94a	2.385[a]	2.471	2.454	2.455
95a	2.443[a]	2.565	2.550	2.551

[a] States are not bound at KT.

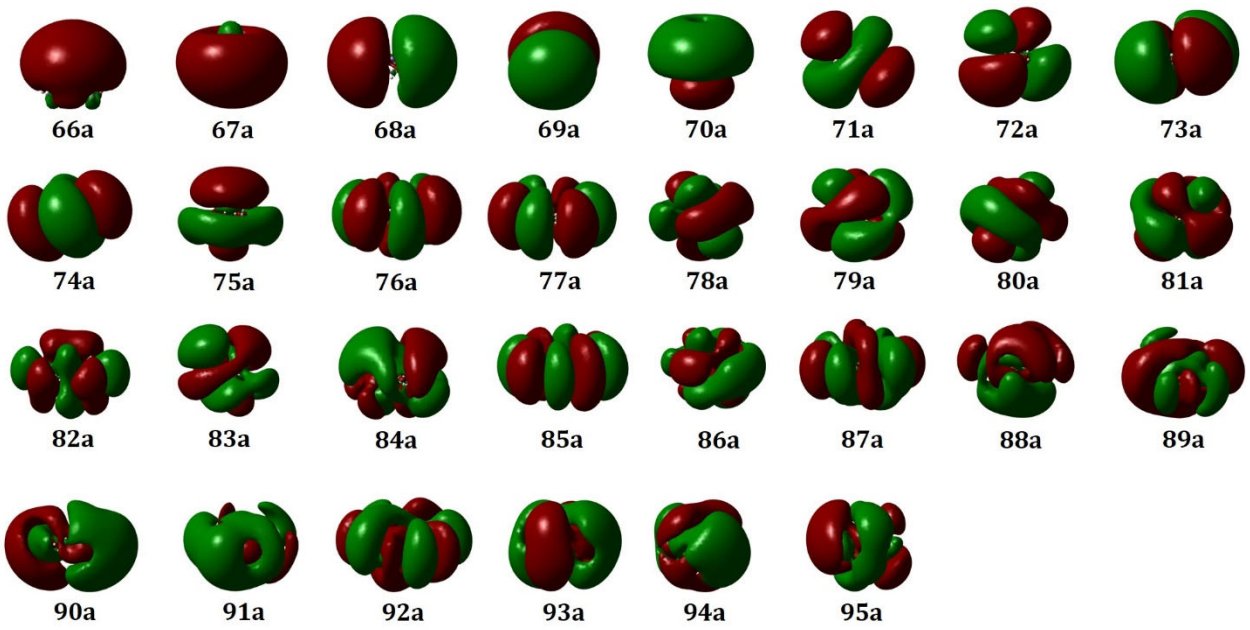

Figure S7. Dyson orbitals for vertical electron attachment to $Na(15C5)^{+}$.

Table S18. Vertical excitation energies (eV) for K(15C5) at the KT, D2, P3, and P3+ levels of theory.

Occupied orbital	H: DADZ, K,C,O: DZ			
	KT	D2	P3	P3+
70a	0.000	0.000	0.000	0.000
71a	0.745	0.774	0.766	0.766
72a	0.816	0.867	0.860	0.860
73a	0.899	0.936	0.926	0.926
74a	1.149	1.236	1.230	1.229
75a	1.166	1.253	1.245	1.245
76a	1.175	1.264	1.256	1.255
77a	1.216	1.301	1.291	1.290
78a	1.217	1.305	1.295	1.295
79a	1.438	1.519	1.521	1.520
80a	1.571	1.692	1.688	1.687
81a	1.593	1.732	1.727	1.726
82a	1.600	1.739	1.733	1.732
83a	1.613	1.751	1.743	1.743
84a	1.618	1.764	1.758	1.757
85a	1.641	1.780	1.775	1.774
86a	1.663	1.779	1.776	1.775
87a	1.886	1.973	1.970	1.970
88a	1.938	2.040	2.038	2.038
89a	2.007	2.184	2.179	2.179
90a	2.015	2.190	2.185	2.184
91a	2.083	2.190	2.186	2.185
92a	2.063	2.193	2.190	2.189
93a	2.048	2.203	2.200	2.199
94a	2.150	2.216	2.211	2.210
95a	2.319	2.382	2.381	2.380
96a	2.304	2.389	2.387	2.386
97a	2.365[a]	2.437	2.436	2.435
98a	2.422[a]	2.492	2.490	2.490
99a	2.522[a]	2.509	2.500	2.500
100a	2.544[a]	2.554	2.547	2.547

[a] States are not bound at KT

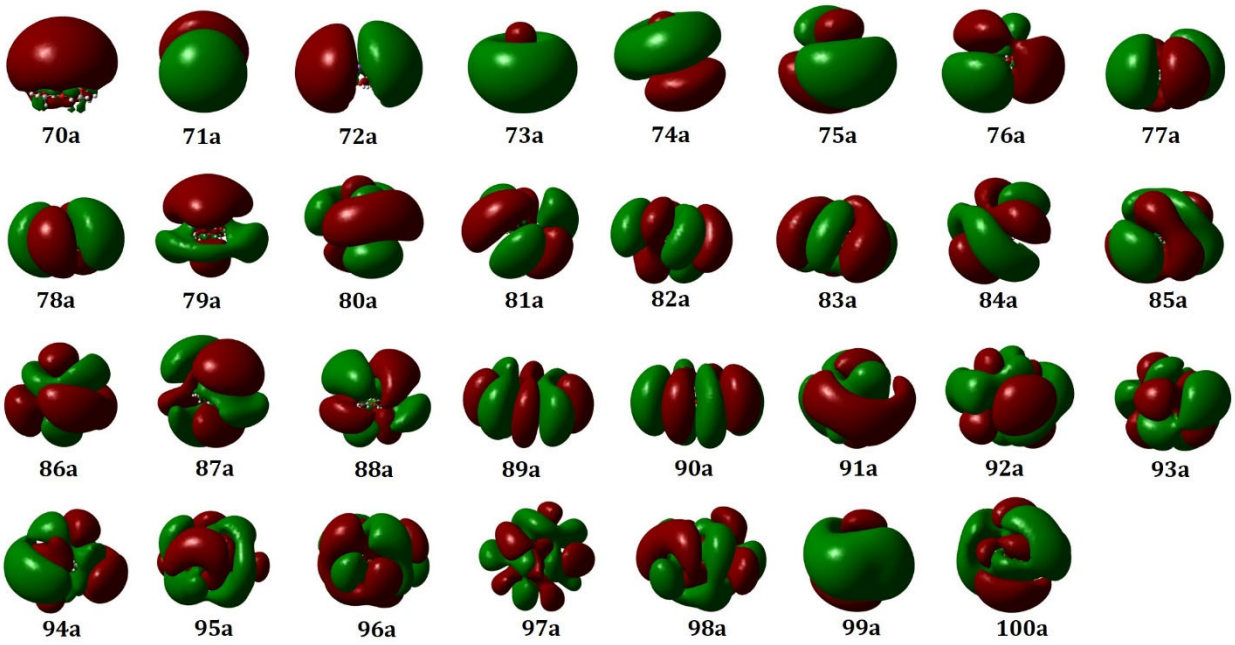

Figure S8. Dyson orbitals for vertical electron attachment to $K(15C5)^+$.

Table S19. Vertical excitation energies (eV) for Na(18C6) at the KT, D2, P3, and P3+ levels of theory.

Occupied orbital	H: DADZ, Na,C,O: DZ			
	KT	D2	P3	P3+
19^2A_1	0.000	0.000	0.000	0.000
20^2A_1	0.550	0.723	0.704	0.706
26^2E	0.578	0.760	0.739	0.741
21^2A_1	0.782	0.958	0.948	0.949
27^2E	0.857	1.081	1.060	1.062
28^2E	0.866	1.094	1.076	1.077
22^2A_1	1.100	1.288	1.283	1.284
10^2A_2	1.183	1.446	1.427	1.429
23^2A_1	1.198	1.462	1.443	1.445
29^2E	1.243	1.523	1.507	1.509
30^2E	1.273	1.559	1.544	1.546
31^2E	1.564	1.871	1.854	1.856
24^2A_1	1.981[a]	1.929	1.942	1.941
32^2E	1.649	1.953	1.940	1.942
11^2A_2	1.631	1.958	1.945	1.946
33^2E	1.878	1.954	1.945	1.946
25^2A_1	2.027[a]	2.053	2.042	2.043
34^2E	2.049[a]	2.155	2.135	2.137
26^2A_1	2.143[a]	2.205	2.189	2.191
35^2E	1.946	2.285	2.272	2.273
36^2E	2.192[a]	2.294	2.274	2.276
12^2A_2	1.992[a]	2.297	2.284	2.285

[a] States are not bound at KT.

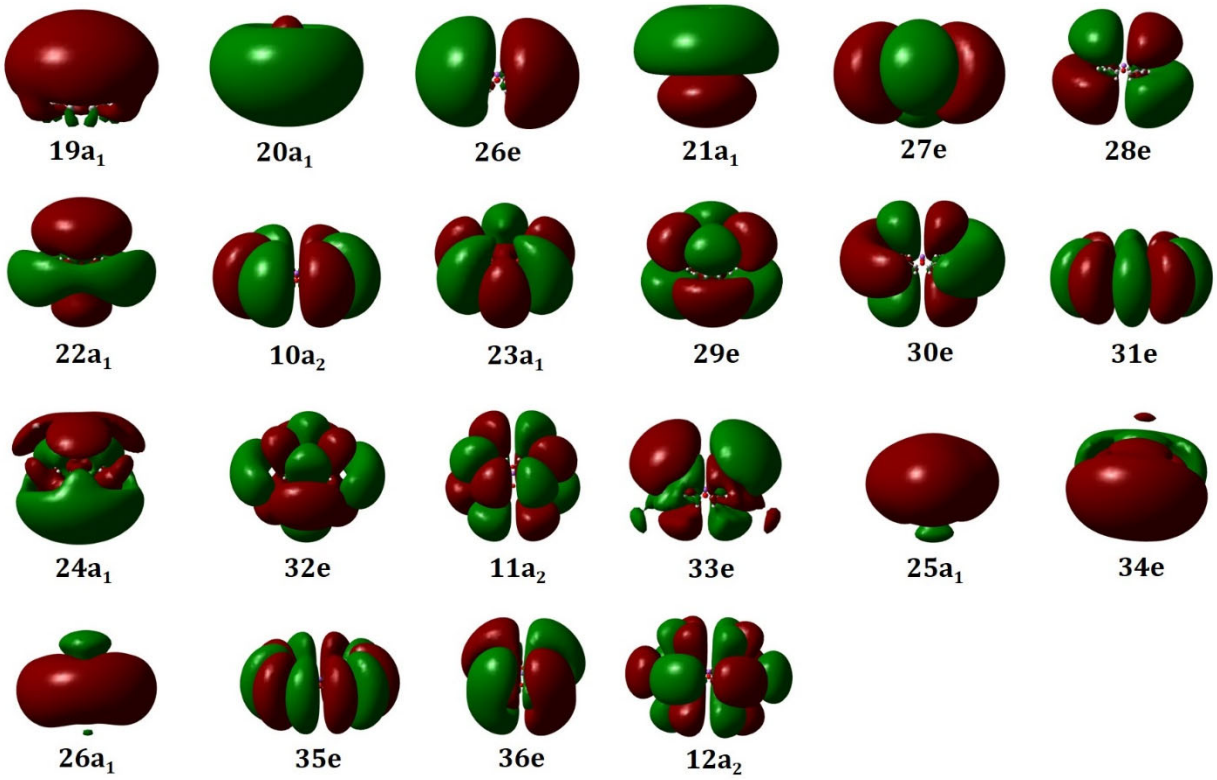

Figure S9. Dyson orbitals for vertical electron attachment to $Na(18C6)^+$.

Table S20. Vertical excitation energies (eV) for K(18C6) at the KT, D2, P3, and P3+ levels of theory.

Occupied orbital	H: DADZ, K,C,O: DZ			
	KT	D2	P3	P3+
21^2A_1	0.000	0.000	0.000	0.000
27^2E	0.627	0.700	0.690	0.691
22^2A_1	0.677	0.761	0.750	0.751
23^2A_1	0.914	1.036	1.031	1.031
28^2E	0.935	1.060	1.051	1.051
29^2E	0.949	1.068	1.056	1.057
24^2A_1	1.235	1.367	1.366	1.366
10^2A_2	1.278	1.439	1.429	1.429
25^2A_1	1.296	1.461	1.450	1.451
30^2E	1.320	1.495	1.489	1.489
31^2E	1.337	1.510	1.504	1.504
26^2A_1	1.689	1.756	1.755	1.755
32^2E	1.703	1.795	1.793	1.793
33^2E	1.658	1.861	1.853	1.854
11^2A_2	1.711	1.933	1.928	1.928
34^2E	1.740	1.934	1.930	1.930
27^2A_1	2.118[a]	1.978	1.994	1.993
35^2E	1.985	2.036	2.028	2.028
36^2E	2.137[a]	2.198	2.191	2.192
28^2A_1	2.240[a]	2.227	2.218	2.218
37^2E	2.037	2.274	2.269	2.269
12^2A_2	2.083[a]	2.283	2.278	2.278

[a] States are not bound at KT.

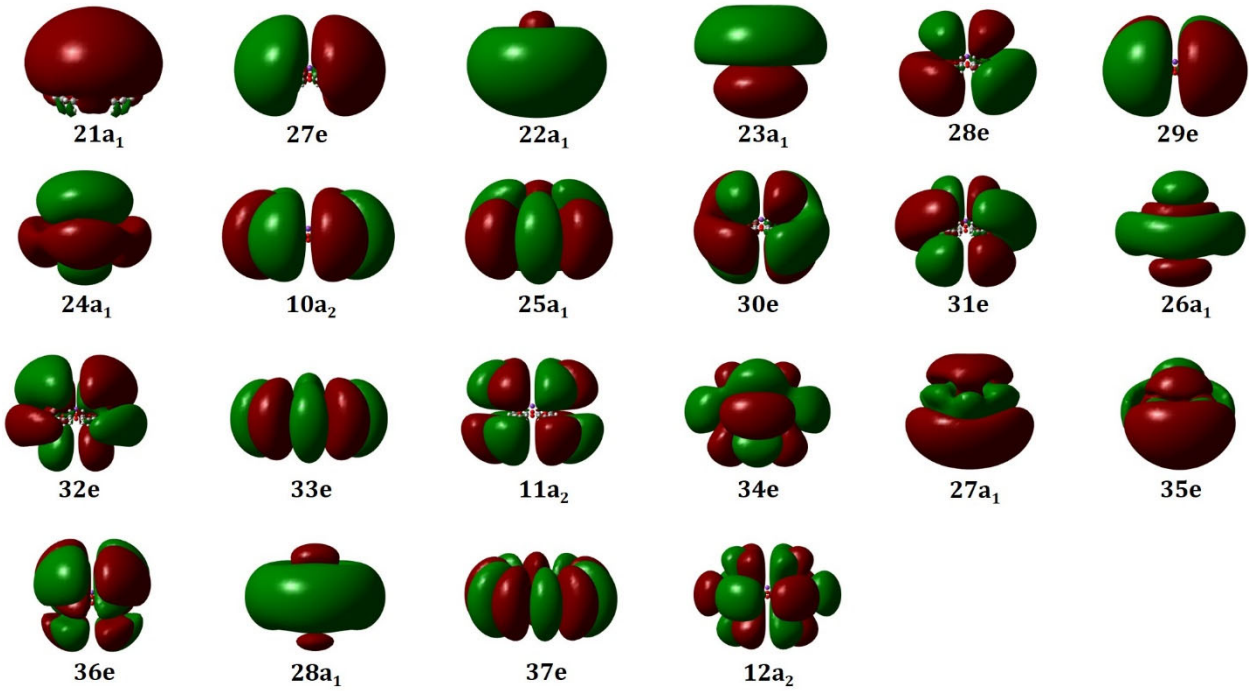

Figure S10. Dyson orbitals for vertical electron attachment to $K(18C6)^+$.

Table S21. CAM-B3LYP optimized geometries (Cartesian coordinates in Å) for $M(12C4)_2$ (M = Li, Na, K).

$Li(12C4)_2$			$Na(12C4)_2$			$L\text{-}K(12C4)_2$			$S\text{-}K(12C4)_2$		
O	1.951106	1.998037	0.269331	O	-1.674954	1.263680	-0.611101	O	0.326633	2.531683	1.700322	O	-1.613187	0.000000	2.992940
O	3.347261	-0.000264	-0.669529	O	-4.562571	1.118070	-0.328696	O	0.248132	4.821037	0.000000	O	0.000000	2.202774	3.941601
O	1.600043	0.000082	1.930411	O	-1.114520	-1.321368	-1.913331	O	2.175971	1.154136	0.000000	O	-0.000000	-2.202774	3.941601
O	1.950434	-1.998109	0.269761	O	-3.210685	-1.377575	0.076441	O	0.326633	2.531683	-1.700322	O	1.613187	0.000000	2.992940
C	1.845262	2.299745	1.657949	C	-0.823169	1.046790	-1.720240	C	1.411966	1.759918	2.167859	C	-2.126777	-1.184481	3.556062
C	3.535467	1.222677	-1.355639	C	-3.765383	2.191164	0.116800	C	-0.471694	4.728718	1.206787	C	-1.208506	2.333853	3.230238
C	1.014783	1.223842	2.327837	C	-0.171947	-0.308602	-1.623488	C	1.676535	0.629459	1.206002	C	-1.208506	-2.333853	3.230238
C	3.535249	-1.223502	-1.355163	C	-4.963354	0.151634	0.618225	C	-0.471694	4.728718	-1.206787	C	1.208506	2.333853	3.230238
C	1.013979	-1.223278	2.327915	C	-1.311674	-2.352743	-0.977020	C	1.676535	0.629459	-1.206002	C	1.208506	-2.333853	3.230238
C	3.207670	-2.302335	-0.345683	C	-4.616438	-1.228973	0.125582	C	0.296599	3.865312	-2.174053	C	2.126777	1.184481	3.556062
C	1.844020	-2.299710	1.658366	C	-2.777517	-2.500110	-0.659677	C	1.411966	1.759918	-2.167859	C	2.126777	-1.184481	3.556062
C	3.208220	2.301979	-0.346507	C	-2.569150	2.349248	-0.785704	C	0.296599	3.865312	2.174053	C	-2.126777	1.184481	3.556062
H	1.389090	3.281700	1.804894	H	-0.050678	1.823197	-1.765115	H	1.200247	1.356350	3.165087	H	-3.130708	-1.396315	3.166635
H	2.840460	2.307238	2.105022	H	-1.405928	1.092699	-2.644273	H	2.309118	2.381179	2.232986	H	-2.195489	-1.082635	4.643643
H	2.884389	1.269140	-2.234498	H	-3.438452	2.037686	1.149993	H	-1.469610	4.310986	1.040499	H	-1.026432	2.361100	2.152118
H	4.571936	1.334428	-1.690096	H	-4.344557	3.119991	0.091869	H	-0.608158	5.721069	1.649683	H	-1.702237	3.271569	3.506062
H	1.056186	1.349024	3.413702	H	0.644361	-0.355104	-2.348997	H	2.402060	-0.058817	1.652295	H	-1.702237	-3.271569	3.506062
H	-0.032322	1.260011	2.012437	H	0.268015	-0.440739	-0.632992	H	0.758369	0.062338	1.029487	H	-1.026432	-2.361100	2.152118
H	4.571748	-1.335654	-1.689424	H	-6.046075	0.207711	0.766531	H	-0.608158	5.721069	-1.649683	H	1.702237	3.271569	3.506062
H	2.884290	-1.270108	-2.234096	H	-4.487408	0.328356	1.587057	H	-1.469610	4.310986	-1.040499	H	1.026432	2.361100	2.152118
H	-0.033033	-1.258920	2.012134	H	-0.756711	-2.157524	-0.055256	H	0.758369	0.062338	-1.029487	H	1.026432	-2.361100	2.152118
H	1.054953	-1.348303	3.413809	H	-0.942751	-3.299233	-1.385094	H	2.402060	-0.058817	-1.652295	H	1.702237	-3.271569	3.506062
H	3.166789	-3.280290	-0.830857	H	-5.056313	-1.976615	0.795636	H	-0.172535	3.911521	-3.162933	H	3.130708	1.396315	3.166635
H	3.986341	-2.321390	0.417957	H	-5.032225	-1.371568	-0.876262	H	1.317154	4.248336	-2.255778	H	2.195489	1.082635	4.643643
H	2.839078	-2.307846	2.105729	H	-3.339657	-2.569828	-1.595490	H	2.309118	2.381179	-2.232986	H	2.195489	-1.082635	4.643643
H	1.387157	-3.281357	1.805215	H	-2.940140	-3.421586	-0.088099	H	1.200247	1.356350	-3.165087	H	3.130708	-1.396315	3.166635
H	3.167261	3.279760	-0.832019	H	-2.063183	3.296349	-0.565697	H	-0.172535	3.911521	3.162933	H	-3.130708	1.396315	3.166635
H	3.987052	2.321277	0.416958	H	-2.912460	2.375644	-1.823240	H	1.317154	4.248336	2.255778	H	-2.195489	1.082635	4.643643
Li	1.568663	-0.000012	-0.004695	Na	-1.646504	-0.084762	1.576016	K	-1.795078	1.495600	0.000000	K	0.000000	0.000000	0.000000
H	-3.691571	-3.098738	-0.112412	H	4.216048	-2.931156	-0.363825	H	0.649261	-3.988228	-3.132432	H	-3.271569	-1.702237	-3.506062
H	-1.329141	-3.091545	-1.369160	H	2.475124	-3.057848	1.800021	H	-1.682274	-2.493611	-3.129832	H	-3.271569	1.702237	-3.506062
C	-3.376312	-2.084412	0.165557	C	3.685618	-1.977692	-0.487532	C	0.698373	-3.562723	-2.121382	C	-2.333853	-1.208506	-3.230238
C	-1.284327	-2.082747	-0.936509	C	2.179033	-2.104372	1.342461	C	-1.290537	-2.264502	-2.129951	C	-2.333853	1.208506	-3.230238
H	-2.831587	-2.146812	1.114739	H	2.818333	-2.153996	-1.133792	H	1.247850	-2.616338	-2.177450	H	-2.361100	-1.026432	-2.152118
H	-0.815397	-2.170837	0.048053	H	1.417290	-2.324772	0.587333	H	-0.633826	-1.392314	-2.225215	H	-2.361100	1.026432	-2.152118
O	-2.562968	-1.522435	-0.831651	O	3.277902	-1.463488	0.753119	O	-0.587188	-3.354488	-1.599134	O	-2.202774	0.000000	-3.941601
C	-4.591276	-1.210790	0.348366	C	4.599994	-0.975778	-1.146517	C	1.436971	-4.510588	-1.210081	H	-1.396315	-3.130708	-3.166635
C	-0.431769	-1.223166	-1.831759	C	1.599275	-1.209777	2.408631	C	-2.441244	-1.935274	-1.214359	H	-1.396315	3.130708	-3.166635
H	-5.321244	-1.739999	0.968006	H	5.090986	-1.446027	-2.004531	H	2.353256	-4.847011	-1.705515	C	-1.184481	-2.126777	-3.556062
H	0.467338	-1.777263	-2.101532	H	0.857758	-1.765020	2.990120	H	-3.109864	-1.224158	-1.708334	C	-1.184481	2.126777	-3.556062
H	-5.044090	-1.023123	-0.627463	H	5.370605	-0.678497	-0.432002	H	0.807999	-5.384010	-1.024852	H	-1.082635	-2.195489	-4.643643
H	-0.982287	-0.998344	-2.743647	H	2.396689	-0.898169	3.083579	H	-3.004452	-2.845987	-1.009432	H	-1.082635	2.195489	-4.643643
O	-4.237971	0.000640	0.978045	O	3.861226	0.145446	-1.577891	O	1.762302	-3.863946	-0.000000	O	-0.000000	-1.613187	-2.992940
O	-0.033501	-0.000545	-1.200620	O	0.977648	-0.071246	1.828983	O	-1.968586	-1.368473	-0.000000	O	0.000000	1.613187	-2.992940
C	-4.590746	1.211866	0.347668	C	4.339891	1.427359	-1.237002	C	1.436971	-4.510588	1.210081	C	1.184481	-2.126777	-3.556062
C	-0.431126	1.222349	-1.831766	C	1.363479	1.203909	2.328294	C	-2.441244	-1.935274	1.214359	C	1.184481	2.126777	-3.556062
H	-5.043003	1.023860	-0.628353	H	5.157684	1.354972	-0.516765	H	0.807999	-5.384010	1.024852	H	1.082635	-2.195489	-4.643643
H	-0.981989	0.997791	-2.743508	H	2.227808	1.102412	2.984783	H	-3.004452	-2.845987	1.009432	H	1.082635	2.195489	-4.643643
H	-5.320968	1.741481	0.966663	H	4.715950	1.931496	-2.132977	H	2.353256	-4.847011	1.705515	O	2.202774	-0.000000	-3.941601
H	0.468270	1.775851	-2.101750	H	0.537268	1.624627	2.909425	H	-3.109864	-1.224158	1.708334	H	1.396315	-3.130708	-3.166635
O	-2.562105	1.522695	-0.831835	O	2.932077	1.725401	0.634737	O	-0.587188	-3.354488	1.599134	H	1.396315	3.130708	-3.166635
C	-3.375467	2.085107	0.165102	C	3.229140	2.248452	-0.631527	C	0.698373	-3.562723	2.121382	C	2.333853	-1.208506	-3.230238
C	-1.283155	2.082371	-0.936453	C	1.711880	2.133354	1.195666	C	-1.290537	-2.264502	2.129951	C	2.333853	1.208506	-3.230238
H	-2.830968	2.147409	1.114421	H	2.350137	2.201413	-1.283888	H	1.247850	-2.616338	2.177450	H	2.361100	-1.026432	-2.152118
H	-0.814297	2.170048	0.048168	H	0.913993	2.111853	0.446106	H	-0.633826	-1.392314	2.225215	H	2.361100	1.026432	-2.152118
H	-3.690284	3.099510	-0.113071	H	3.543842	3.298412	-0.562982	H	0.649261	-3.988228	3.132432	H	3.271569	-1.702237	-3.506062
H	-1.327379	3.091257	-1.368951	H	1.779128	3.158725	1.582862	H	-1.682274	-2.493611	3.129832	H	3.271569	1.702237	-3.506062

Table S22. Vertical excitation energies (eV) for S-K(12C4)$_2$ at the KT, D2, P3, and P3+ levels of theory.

Occupied orbital	Excitation energy (eV)			
	KT	D2	P3	P3+
$1a_1$	0.000	0.000	0.000	0.000
1e	0.402	0.654	0.633	0.635
$2a_1$	0.731	1.066	1.055	1.057
$1b_2$	0.783	1.168	1.146	1.148
$1b_1$	0.779	1.169	1.147	1.149
$2b_2$	0.881	1.323	1.303	1.305
2e	0.996	1.450	1.429	1.431
3e	1.081	1.445	1.431	1.433
$3a_1$	1.094	1.534	1.523	1.524
$1a_2$	1.247	1.736	1.717	1.718
4e	1.243	1.744	1.725	1.727
$4a_1$	1.286	1.770	1.751	1.752
$3b_2$	1.325	1.809	1.794	1.795
5e	1.406	1.857	1.845	1.846